

Zeitschrift: Helvetica Physica Acta
Band: 62 (1989)
Heft: 2-3

Vereinsnachrichten: Rapport de la réunion d'automne de la Société Suisse de Physique
des 6 et 7 octobre 1988 à Lausanne

Autor: [s.n.]

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REUNION D'AUTOMNE DE LA SOCIETE SUISSE DE PHYSIQUE
DES 6 ET 7 OCTOBRE 1988 A LAUSANNE

TITRES DES COMMUNICATIONS

*P = publié dans le fascicule (4 pages)

Matière condensée

*P

Destruction de l'état mixte à deux dimensions (M) dans les couches cylindriques minces supraconductrices de Type I
E.Holguin, B.Dutoit, G.Burri, R.Schöpfer et L.Rinderer
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Etude magneto-optique dynamique de l'état intermédiaire
B.Dutoit, L.Rinderer, Institut de physique expérimentale,
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Thermische Leitfähigkeit und spezifische Wärme von $U_{(1-x)}Th_xBe_{13}$
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Two-dimensional modulated arrays of Josephson junctions: searching for the Ising transition
R.Théron, R.Rentsch, J.Gavilano, Ch.Leemann and P.Martinoli,
Institut de Physique, 2000 Neuchâtel, Switzerland

Electronic properties and critical current densities of superconducting $(Y_1Ba_2Cu_3O_{6.9})_{1-x}Ag_x$ Compounds
D.Pavuna, H.Berger, M.Affronte and J.Van der Maas,
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J.J.Capponi, M.Guillot, P.Lejay and J.L.Tholence, Centre National de la Recherche Scientifique, B.P.166, F-38042 Grenoble

Magnetic Properties of Crystalline and Amorphous Bi-Ca-Sr-Cu-O
G.Leemann, H.Jenny, H.P.Lang, T.Frey, and H.-J.Güntherodt

Complex ac Conductance of YBaCuO Films
P.K.Srivastava*, P.Debély*, H.E.Hintermann*, Ph.Flückiger+,
J.L.Gavilano+, Ch.Leemann+, J.Weber+ and P.Martinoli+
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Ceramic Oxide Films Produced by Spray Pyrolysis
S.P.S.Arya*, H.E.Hintermann*, D.Morel*, Ph.Flückiger+, J.Weber+
and P.Martinoli+, *CSEM, CH-2000 Neuchâtel
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Total-energy electronic-structure calculations for ordered Fe-Ni compoundsT.Jarlborg*, E.G.Moroni

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Relationship between electronic conduction states and indirect magnetic exchangeP.Monachesi*, P.Giannozzi^O*, M. Acquarone[^]

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^O IRRMA, EPFL, 1024 Ecublens[^]Dipartimento di Fisica, Università di Parma, 43100 Parma (Italy)**Electronic susceptibility and electron-phonon coupling of ScN**M.M. Steiner and R.Monnier, Laboratorium für Festkörperphysik, ETH-Hönggerberg, CH-8093 Zürich; D.D. Koelling, Argonne National Laboratory, Argonne, Illinois 60439, USA**Electronic structure and XPS spectra of disordered Hf carbonitrides**G.H.Schadler and R. Monnier, Laboratorium für Festkörperphysik, ETH-Hönggerberg, CH-8093 Zürich**Elektronische Eigenschaften von Ca_3Pd_2 und Ca_3Pd_2 -Hydrid**L.Schlapbach, Inst. de Physique, Université, CH-1700 Fribourg
J.P. Burger, Université Paris-Sud, F-91405 Orsay**Analyse de la surface de getter par XPS**I.Vedel, L. Schlapbach, Inst. de Physique, Université Fribourg, CH-1700 Fribourg

*p

Optische und magnetooptische Messungen an einkristallinem NdSH.Brändle, J.Schoenes und F.Hulliger, Festkörperphysik, ETH-Zürich

*p

Optische Eigenschaften von EuMo_6S_8 P.Fumagalli, J.Schoenes und O. Fischer*, Lab. für Festkörperphysik, ETH-Zürich, *Dép. de Physique de la Matière Condensée, Université de Genève

*p

Hall-Effekt von UCuP_2 und UCu_2P_2 N.Korner, J.Schoenes und D.Kaczorowski*, Festkörperphysik ETHZ

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Pouvoir thermoélectrique de CeInCu_2 A.Basset, D.Jaccard et J.Sierro

DPMC, Université de Genève, 24, quai E.-Ansermet, 1211 Genève 4

Rôle de la phase liante dans les propriétés mécaniques du métal dur WC-Co étudié par frottement intérieur

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Déformation à haute température du métal dur WC-Co

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Mesures localisées par Microscopie Acoustique des propriétés élastiques en tête de fissures dans du WC-CoA.Kulik, S.Satish, G.Gremaud, D.Mari, EPFL, Dépt. de physique, Institut de génie atomique, CH-1015 Lausanne**Inhomogene Verteilung weitreichender innerer Spannungen in ermüdeten Cu-Einkristallen**T.Ungár*, I.Puppán und S.Stanzl**

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Far infrared reflectivity measurements on quasi-one-dimensional halogen-bridged mixed-valence compounds

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M.Haruki and S.Kurita, Yokohama National University, Lab.of Applied Physics Hodogava, Yokohama 240, Japan

*p

Inelastic light (Raman) scattering from strained ultra-short period SiGe superlatticesW.Bacsa, M.Ospelt, J.Henz, K.A.Mäder, H.von Känel and P.Wachter, Laboratorium für Festkörperphysik, ETH Zürich, 8093 Zürich**Fracton Interpretation of the Specific Heat of Styrcast**E.Felder, T.Sleator, A.Bernasconi, H.R.Ott, Laboratorium für Festkörperphysik, ETH-Hönggerberg, 8093 Zürich, Switzerland

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Fluctuations de densité à l'interface solide-liquide du cyclohexaneE.Steininger et J.Bilgram,

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Electronic properties of (GaAs)_n(AlAs)_n(001) superlattices and band offsets in GaAs/AlAs heterojunctions

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Schwere-Kapillar-Wellen kleiner Amplituden über suprafluidem Helium II endlicher Tiefe

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Durch Zweiten Schall erzwungene nichtlineare**Schwere-Kapillar-Wellen**

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Grenzflächeneigenschaften und Adhäsion von a-C:H Filmen auf GaAs(100)

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Adsorption von Wasser auf Ni, Zr und amorphem Ni₆₄Zr₃₆

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Surface investigations of donor graphite intercalation compounds by scanning tunneling microscopy (S T M)

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Bombardement ionique avec des ions d'iode: effet en surface

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Geometrical and electronic structure of neutral, positively and negatively charged Magnesium clusters

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Matrix deposition of neutralized, mass selected silver atoms and clusters

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Dislocation loop formation by electron irradiation in aluminium

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Propriétés Mécaniques et Microstructure d'une Phase $L1_2$ Pure Monocristalline de Composition $Ni_3(Al,1\%Ta)$

N.Baluc, Institut de Génie Atomique, EPFL, CH-1015 Lausanne

Stades de durcissement de monocristaux de cuivre d'axe (112) aux intermédiaires et hautes températures

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Microscopie électronique en transmission du nouveau catalyseur à base de Na_2MoO_4 pour une production de formaldéhyde en l'absence de H_2O

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Growth of bubbles during annealing of 600 MeV proton irradiated aluminium

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Untersuchungen zur Struktur der Korngrenzen in Korund

Hans Grimmer, Paul Scherer Institut, CH-5303 Würenlingen

Highly Dispersed Heterogeneous Catalysts by Physical Vapour Deposition (PVD)

J.P.Bucher, M.Flüeli and J.J.van der Klink

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Etude RMN du Ta dans les systèmes $KTaO_3$ purs et dopés

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Photoemissionsmessungen an flüssigem Lithium

G.Indlekofer, P.Oelhafen und H.-J.Güntherodt

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Surface Oxidation of Amorphous Ni - Zr Alloys

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Neutronenspektroskopie an quasikristallinem und amorphem

$\text{Pd}_{58.8}\text{U}_{20.6}\text{Si}_{20.6}$

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Small angle neutron scattering from coherent precipitates with variable lattice mismatch

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Entmischung von Ni-Ti-Einkristallen

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Amorphisierungsreaktionen in Nb-basierten Legierungen

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Silicide Formation for Cu on a-Si:H

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Macroscopic Quantum Tunneling and Thermal Activation in Small-Area Josephson Tunnel Junctions and dc-SQUIDS

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Physique appliquée

Oxygen Ionosorption/Desorption on Doped (Ar, Pd) thin SnO₂ Gas Sensor

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Echtzeit-Röntgen-Mikroskopie: Der Röntgen-CCD

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Programme G³ pour le calcul de systèmes solaires actifs

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Evaluation du rayonnement solaire sur un plan incliné à partir de sa connaissance sur un plan horizontal

P. Ineichen, A. Zelenka*, O. Guisan, A. Razafindraibe

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Detection and Destruction of Malignant Tumors with Light and Porphyrins

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Lokale Beweglichkeit einer Polymerkette beim Phasenübergang

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XPS Study of Amino Acid Adsorption to Titanium Surfaces

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Computer Model of the Motor-Neural System of a simple Invertebrate

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Extremal properties of dendritic patterns: biophysical applications

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Zur Physik des Denkakts

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Water-Fat Image: A classification Pixel by Pixel

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Morphology and structure of TiSi_2 thin films on Silicon

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Le rôle de l'oxygène lors de la formation des couches minces de TiSi_2 par recuit rapide

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Sputtered black decorative coatings based on Ti-Al-O-N

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Structural Characterization of ultra-short period Si-Ge superlattices

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Parallel Electric Transport in Thin CoSi_2 Layers on Si(111)
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BaF_2 - SrF_2 (100) Schichten mit glatter Oberfläche auf Si (100)

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Photovoltaische Infrarotsensoren auf Silizium Substraten

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Band-filling effect in bulk and quantum wells GaAs/Al_xGa_{1-x}As phase modulators

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Photoluminescence of disordered AlGaAs/GaAs quantum wells via Zinc diffusion

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Résistance de caisson: mesure, modèle et simulation

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Properties of hydrodynamic systems with flexible boundary conditions

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Resonant stimulation and control of Karman's vortex street

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Resonant stimulation and control of a nonlinear mechanical pendulum by Poincaré maps

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Formation of Selfsimilar Dendritic Patterns with Extremal Properties

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Digital temperature controller for low temperature experiments
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Bedingte Entropie: Eine neue Methode zur Konstruktion optimaler neuronaler Netzwerke

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Efficient image compression for electronic mail transmission

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Aufladung von Aerosolen in ionisierten Gasen

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Nucleation in supercooled metals with high melting point

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Einfluss von Relaxation und Ionenbeschuss auf elektr.Eigenschaften von Au/Si-Schichten

H.-G. Boyen, P.Rieger, P.Häussler, F.Baumann
(Phys.Inst.Univ.Karlsruhe) G.Indlekofer, P.Oelhafen,
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Boundary thermal conductances in liquid helium deduced from normal phase propagating velocities along superconducting wires

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Berry's Phase in Optical Resonance

D.Ellinas, S.M.Barnet and M.A.Dupertuis

Multiatom Quasi-intelligent and Squeezed States

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Amplification d'un mode faible dans un laser vibronique à plusieurs modes

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F.Schwendimann, Groupem. p.l'armement, Kasernstr.19, 3000 Bern 25

Neuer integriert-optischer Modulator

P.Pliska, V.Briguet und W.Lukosz, Prof. f. Optik, ETH, 8093 Zürich

Experimentelle Untersuchungen der durch thermische Ausdehnung bewirkten optischen Bistabilität von Fabry-Perot-Etalons

G.Appenzeller-Combe, P.Pirani und W.Lukosz

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Effizientes Einkoppeln von Laserlicht in Fiberbündel

S.Wüthrich, W.Lüthy und H.P.Weber; Inst.für angewandte Physik, Universität Bern, Sidlerstrasse 5, 3012 Bern

Fokussieren am Ausgang eines phasengesteuerten Fiberarrays

G.Josten, H.P.Weber und W.Lüthy; Inst. für angewandte Physik, Universität Bern, Sidlerstrasse 5, 3012 Bern

Thermisches Verhalten von Linienbreite und -position von Fluoreszenzlinien in YALO:ER3+

C.Pfistner, P.Albers, W.Lüthy und H.P.Weber;

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Mesure du diamètre moyen de bulles de gaz par la méthode de l'écart-type

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The Impact of Neutral Networks on Tokamak Control

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Numerical calculation of electrical breakdown in oxygen in a dielectric-barrier discharge

W.Egli and B.Eliasson, ASEA Brown Boveri, Corporate Research, 5405 Baden, Switzerland

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On the theory of Z-pinch in a dense plasma

Yu.S.Sayasov, Institute of Physics, University of Fribourg, 1700 Fribourg, Switzerland

Astrophysique, Physique nucléaire et corpusculaire

The $d + p \rightarrow {}^3\text{He} + \eta$ reaction at threshold

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Effet inattendu dans le transfert de muons négatifs dans un mélange gazeux de $\text{H}_2 + \text{SO}_2$

R.Jacot-Guillarmod, F.Mulhauser, P.Oberson, C.Piller,
L.Schellenberg et H.Schneuwly

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Polarization transfer measurements in p-d-scattering at 22.7 MeV

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Analyse de fonctions de réponse d'un détecteur à neutrons NE213

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Comparison of inclusive production cross-sections of π^0, η, γ and J/ψ in pp and $p\bar{p}$ interactions at $\sqrt{s} = 24,3 \text{ GeV}$.

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Search for the Rare Decay $K^+ \rightarrow \pi^+ \mu^+ e^-$

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Law of constant passion and inertia of the cosmic distance

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Vorschlag zum Bau von Elektron-Positron Speicherringen für Teilchenphysik mit schweren Quarks und Leptonen sowie Synchrotronstrahlung

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Is gravitational energy-momentum really non localizable?

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Transformation to Normal Time for the Calculation of Poincaré Maps in a Closed Form

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Adaptive control of chaotic systems

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Description of the Dynamics of Extended Nonlinear Systems by Analytically Calculated Operators

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Cooling-Rate Dependence of the Residual Energy of a One-Dimensional Structural Glass Model

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Délocalisation phononique dans les semiconducteurs amorphes

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Why Do "Dirty" Tips Produce Higher Resolution Images When Scanning Graphite in a Scanning Tunneling Microscope?

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Critical current and magnetization of ceramic high- T_c superconductors

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R.G. Study of some vectoriels and non-linear σ -models

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Bethe lattices and inverse orbits

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Grey Noise and Fractional Diffusion

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Cantor Spectrum and Singular Continuity for a hierarchical Hamiltonian

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Dépendance en température de la résistivité électrique dans le système $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ sous l'action d'un champ magnétique

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DESTRUCTION DE L'ETAT MIXTE A DEUX DIMENSIONS (M) DANS LES
COUCHES CYLINDRIQUES MINCES SUPRACONDUCTRICES DE TYPE I

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Nous présentons une étude théorique et expérimentale réalisée dans des couches cylindriques minces d'étain. La présence de l'état M dans ces échantillons semble expliquer la forme des caractéristiques courant-tension. Une attention particulière est portée sur le domaine proche du courant de destruction de l'état M que nous évaluerons très précisément. L'ordre de grandeur de son épaisseur est également donné.

1. INTRODUCTION

L'existence de l'état M dans les supraconducteurs cylindriques creux de type I a été postulé en 1938 par L.D. Landau et différentes études théoriques ¹ et expérimentales ² ont été réalisées. Ces travaux montrent notamment que cet état est formé de domaines supraconducteurs et normaux formant une configuration stable dont l'épaisseur serait de l'ordre de la longueur de cohérence. De plus, sa résistance est voisine de zéro.

Le but de ce travail est de montrer que la forme des caractéristiques courant-tension dans les couches cylindriques minces peuvent s'expliquer par sa présence. Ainsi que nous le verrons, la destruction de cet état a pu être obtenue grâce à la forte densité de courant existant dans l'échantillon que nous calculerons très précisément. En guise de conclusion, nous mentionnerons les difficultés rencontrées à partir du modèle théorique afin d'évaluer son épaisseur.

2. THEORIE

Considérons un fil cylindrique creux parcouru par un courant $I_0 > I_c$, I_c étant le courant critique, et dont les surfaces in-

terne et externe se trouvent aux distances axiales r_1 et r_2 , respectivement. D'après³, le saut ΔE que subit le champ électrique lorsque l'état M vient d'être détruit quand $I_0 = I_m$ (courant de destruction) vaut:

$$\frac{\Delta E}{\Omega_N I_c} \cong - \frac{2r_1 \xi I_m}{(r_2^2 - r_1^2 - 2r_1 \xi) I_c} + \frac{(r_2^2 - r_1^2)(r_1 + \xi)}{(r_2^2 - r_1^2 - 2r_1 \xi) r_2} \quad (1)$$

où ξ et Ω_N sont l'épaisseur de l'état M et la résistance de l'état normal par unité de longueur, respectivement.

Dans le cas des couches minces, c'est-à-dire lorsque $r_2 \rightarrow r_1 + \xi$, cette équation possède une limite inférieure pour I_m . En effet, pour de tels échantillons l'état intermédiaire est pratiquement inexistant et de ce fait la quantité réduite $\Delta E / \Omega_N I_c \rightarrow 1$, car elle prend sa valeur maximale. Ces limites montrent que le courant I_m est fortement réduit et proche du courant critique. En calculant, on trouve:

$$I_m \cong I_c \quad (2)$$

D'autre part, le calcul des caractéristiques courant-tension montre que l'on peut distinguer deux grandes régions. Avant le saut et pourvu que l'épaisseur de l'état M soit très inférieur à celui de la couche cylindrique mince, appelé ϵ , le champ électrique E a pour expression:

$$\frac{E}{\Omega_N I_c} \cong \frac{\epsilon}{\epsilon - \xi} \left(i_0 - \frac{r_1 + \xi}{r_1 + \epsilon} \right) \quad (3)$$

où l'on a posé $i_0 = I_0 / I_c$. Par contre, après le saut, le champ électrique correspond à celui de la courbe de l'état normal.

3. EXPERIENCE

Les Figs. 1 et 2 montrent quelques résultats expérimentaux (points noirs) obtenus sur un même échantillon pour différentes températures T_B du bain d'hélium. La couche cylindrique mince a été réalisée par évaporation de l'étain sur un fil de quartz tournant dont le diamètre été $\phi_1 = 0.356$ mm. Ce procédé garantit l'isolation électrique et un bon contact thermique. L'épaisseur

d'étain ainsi évaporé a été de $\epsilon = 18.61 \text{ KÅ}$.

La courbe de l'état normal (points carrés non remplis) a été réalisée en appliquant un champ magnétique longitudinal suffisamment intense afin de détruire la supraconductivité.

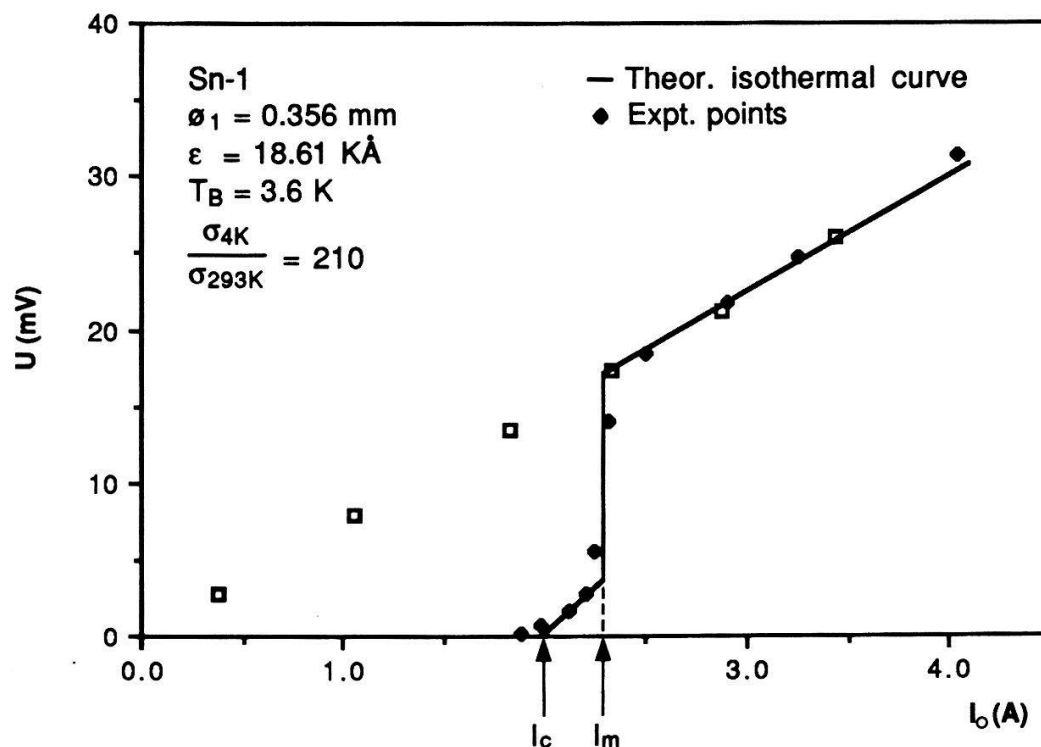


Fig.1 Caractéristique I_0 -U. L'état M est détruit pour $I_m = 2.28 \text{ A}$, ce qui correspond à une densité de courant $j_m = 1.1 \times 10^5 \text{ A./cm}^2$.

Ces figures montrent clairement que la sortie de l'état supraconducteur se fait en "douceur"; c'est-à-dire, sans saut apparent de la tension U. Les points expérimentaux sont alors plus ou moins alignés suivant une droite presque parallèle à la courbe de l'état normal. Cet effet peut être expliqué par la présence de l'état M dans l'échantillon qui porte un courant constant $I_M \approx I_c$. Le décalage de la tension par rapport à la courbe de l'état normal s'explique par le fait que ce courant circule pratiquement sans résistance. Néanmoins, une fois que le courant atteint la valeur $I_0 = I_m$, l'état M est détruit et l'échantillon devient entièrement normal. La Fig.2 montre en particulier que les points expérimentaux peuvent démarrer avant I_c . Ce phénomène

peut être attribué à des transitions thermiques longitudinales. La relation (3) permet d'obtenir des épaisseurs de $\xi = 4.9 \text{ KÅ}$, pour $T_B = 3.6 \text{ K}$, et de $\xi = 2.6 \text{ KÅ}$, lorsque $T_B = 3.4 \text{ K}$, pour l'état M.

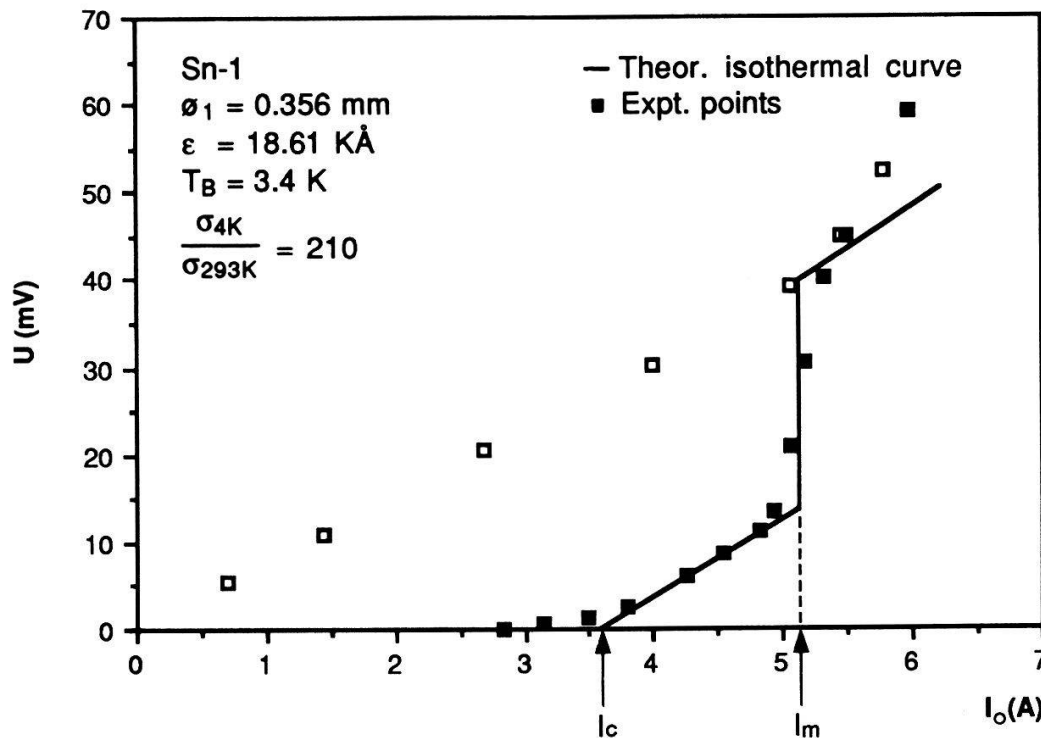


Fig.2 Au moment de la destruction de l'état M, la densité de courant était $j_m = 2.46 \times 10^5 \text{ A/cm}^2$.

Ainsi que le montre la même figure, au-delà de I_m les points expérimentaux tendent à s'éloigner de plus en plus de la courbe théorique isotherme. Pour ces courants, les effets thermiques et de magnétostriction peuvent en être la cause.

4. CONCLUSION

La théorie développée semble expliquer de manière satisfaisante les comportements généraux des caractéristiques I_0 - U dans ces couches cylindriques minces. De même, le courant de destruction I_m a pu être trouvé dans l'expérience très précisément. Par contre, en raison de la difficulté à évaluer des faibles écarts de pente par rapport à la courbe de l'état normal, le calcul de l'épaisseur de l'état M doit être pris avec précaution.

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ETUDE MAGNETO-OPTIQUE DYNAMIQUE DE L'ETAT INTERMEDIAIRE.

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L'enregistrement vidéo de structures d'état intermédiaire dynamique est désormais possible grâce à l'utilisation de couches magnéto-optique au Selenure d'Europium. La rotation spécifique de EuSe est à peu près double de celle du sulfure d'Europium, et plus de quatre fois plus élevée que celle du mélange traditionnel EuS-EuF₂.

Cette plus grande rotation Faraday nous permet de choisir l'angle entre polariseur et analyseur légèrement différent que $\pi/2$, et donc d'augmenter l'intensité lumineuse sur le détecteur.

Ces observations sont menées simultanément avec des mesures des caractéristiques courant-tension, il est dès lors possible de corrélérer ces tensions avec des vitesses de tubes de flux ou de structure.

1. Introduction.

La méthode d'observation magnéto-optique de l'état intermédiaire introduite par Alers (1) utilisait des verres au phosphate de cérium. Par la suite Kirchner (2) remplaça ces verres par des films d'un mélange de sulfure et de difluorure d'Europium. EuS, la substance optiquement active, présente le défaut de prendre un ordre ferromagnétique en dessous de 16.3 K. Cet état influence la structure du superconducteur, et est donc inutilisable pour notre expérience. La dilution avec EuF₂ détruit cet ordre. Laeng (3) a déterminé expérimentalement les meilleures proportions: 0.4 EuS pour 0.6 EuF₂, ce qui produit la plus grande rotation Faraday sans ferromagnétisme. Ce mélange a l'inconvénient de se distiller lors de l'évaporation à cause de la très grande différence de température de sublimation. Zweiacker (4) a affiné la méthode d'évaporation par la confection de pilules du mélange, et par évaporation successive de 50 de ces pilules environ pour obtenir une couche utilisable.

Parmi les sels de terres rares ceux d'europium présentent la plus grande constante de Verdet; en particulier le selenure d'Europium dont la constante est à peu près double de celle du sulfure d'europium, ou quadruple de celle du mélange EuS-EuF₂, ceci toujours à la longueur d'onde de 546 nm utilisée pour l'observation.

		EuS	EuSe	EuS-EuF ₂
V	deg/KOe * μm	4.8	9.6	2.0
μ	μm^{-1}	12	10	4

Constante de Verdet V et coefficient d'absorption μ à 546 nm.

EuSe est métamagnétique et présente un comportement très compliqué à basse température. Dans nos conditions expérimentales, soit un champ limité à 0,5 KOe, nous n'observons pas l'apparition d'un ordre ferromagnétique. Il est donc possible d'utiliser le selenure d'europium à l'état pur, ce qui permet de diminuer l'épaisseur de la couche active à $5 \lambda/4$ nous donnant par conséquent plus de résolution spatiale et moins d'absorption.

2. Technique expérimentale.

Le Selenure d'Europium est sublimé dans un creuset de tantale chauffé par effet joule, sous une pression de 10^{-6} mBars. Le film est déposé directement sur la

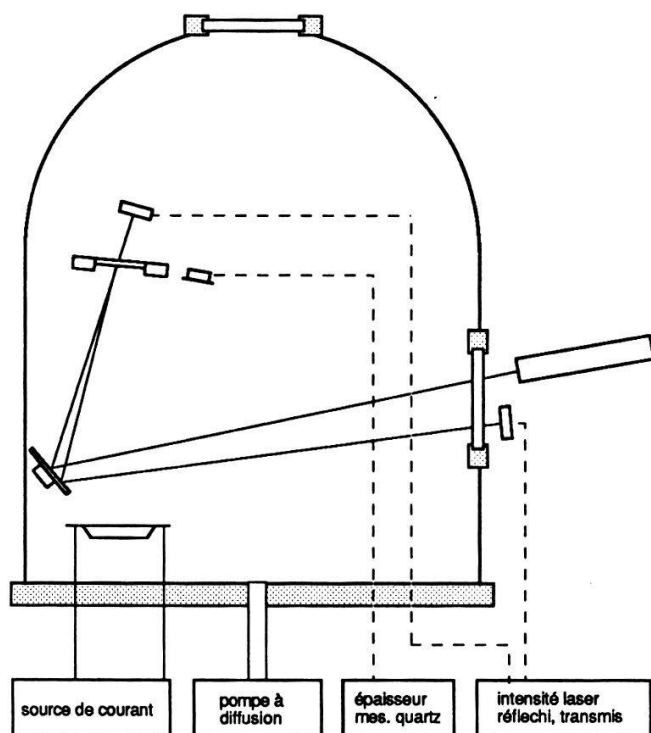


Figure 1.
Installation d'évaporation.

fenêtre froide du cryostat, constituée de verre Schott & Gen SF 57 collé sur une membrane inox 0.1 mm en U elle même soudée sur une bride. Ce montage permet d'absorber la dilatation différentielle lors du refroidissement. Ce verre est choisi en raison de sa faible constante photoélastique, de manière à éviter toute dépolarisation de la lumière lorsque le verre est sous contrainte. Notons au passage que la colle avec laquelle est monté le verre sur sa flasque nous interdit de chauffer la fenêtre lors de l'évaporation, ce qui aurait pour effet d'accroître le pouvoir rotatoire de la couche(5).

Comme nous le voyons sur le schéma ci-contre, trois mesures sont faites pendant l'évaporation:

- épaisseur optique par réflexion,
- épaisseur "massique" par déposition sur un quartz,
- absorption optique.

De plus l'épaisseur mécanique totale de la couche est mesurée par la hauteur du step produit sur un support de verre partiellement masqué durant l'évaporation.

La déposition sur un quartz modifie sa fréquence de résonance par modification de sa masse par unité de surface; il est dès lors possible de connaître l'épaisseur déposée en prenant une masse spécifique de 6 g/cm^3 pour le Sélénure d'euprémium.

Afin d'obtenir un contraste maximum, la couche magnéto-optique doit être une couche anti-reflet pour le miroir aluminium que nous déposons dessus. Pour ce faire, il suffit de cesser l'évaporation lorsque l'épaisseur optique atteint un multiple entier impair de la longueur d'onde. Ceci est faisable grâce à l'enregistrement de l'intensité du rayon laser 543.5 nm. réfléchi en fonction de l'épaisseur mesurée au quartz pendant l'évaporation.

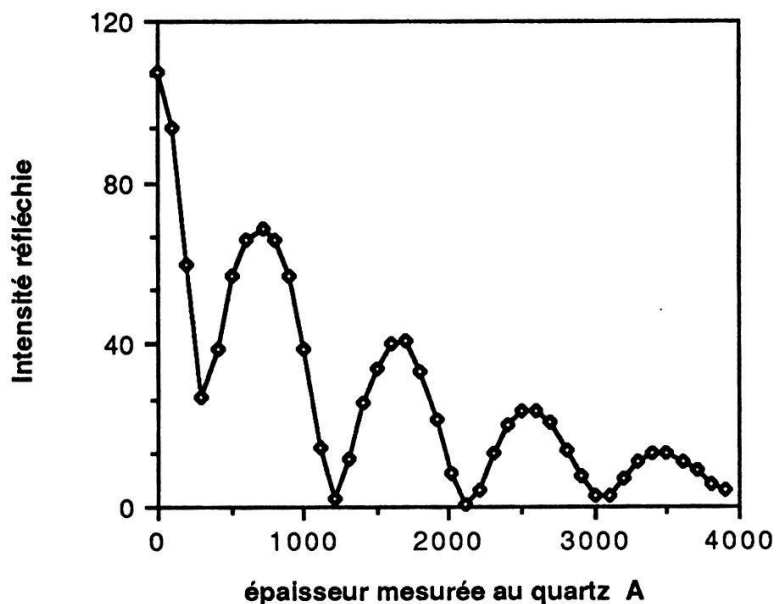


Figure 2.
Intensité lumineuse réfléchie en fonction de l'épaisseur mesurée avec le quartz. (laser 543.5 nm.)

3. Appareillage Optique.

Le système optique est construit autour d'un microscope stereoscopique Wild & Leitz M5 modifié de telle sorte que nous utilisons un côté pour l'éclairage et l'autre pour l'observation. La source de lumière est une lampe à vapeur de mercure de 400 watts soigneusement filtrée ultraviolet et infrarouge. Nous disposons ensuite d'un diaframe de champ puis d'un filtre interférentiel sélectionnant la raie verte du mercure à 546 nm. Un diaframe d'intensité a été incorporé au corps de microscope. Le filtre polariseur se trouve placé juste avant l'entrée du faisceau dans le cryostat, à travers successivement les fenêtres à température ambiante et à l'azote. L'analyseur se trouve juste à la sortie du cryostat, le microscope nous renvoyant l'image dans le viseur ou dans le détecteur vidéo ou photographique.

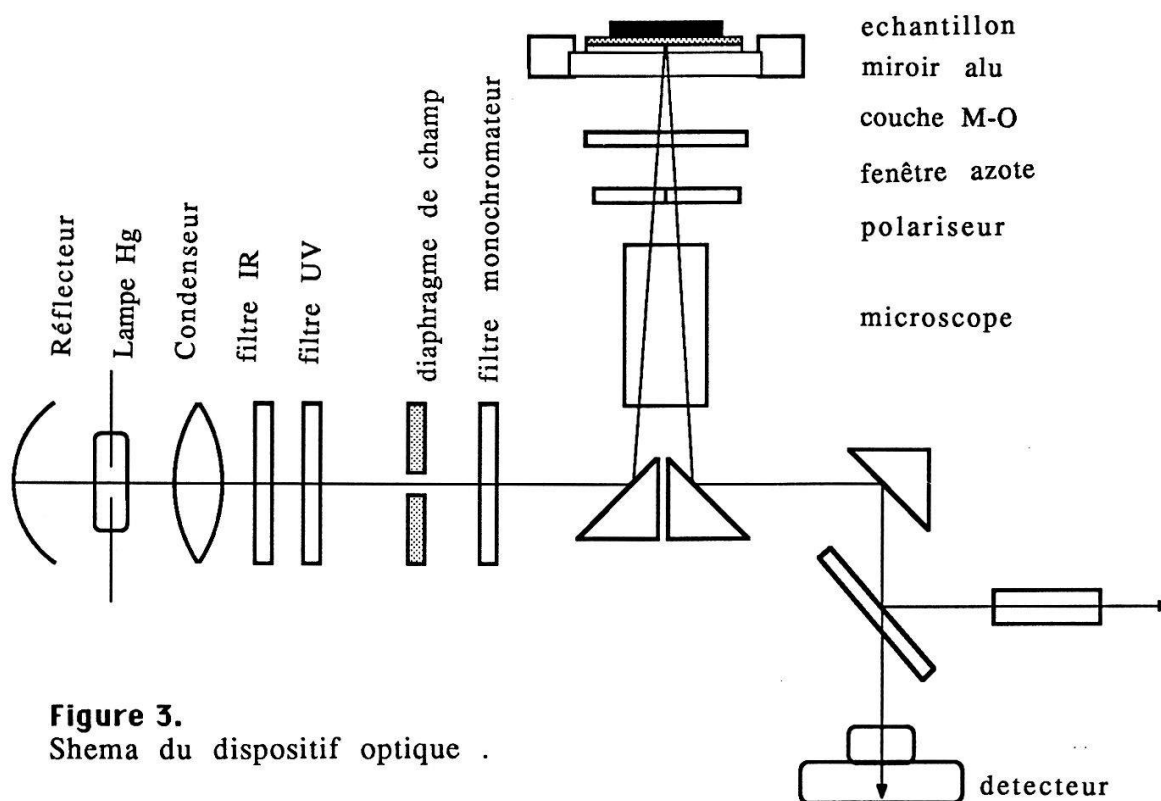


Figure 3.
Schéma du dispositif optique .

Il est possible de prendre des vues statique sur du film tri-X pan 35mm que l'on pousse deux fois lors du développement. Les vues dynamiques sont possibles soit grâce à une camera 16mm, mais à des vitesses lentes de l'ordres de 2 à 6 images par seconde, soit avec une camera vidéo couplée à un intensificateur d'image.

Cette dernière a l'avantage de produire des images directement vérifiables et utilisables. De plus il devrait être possible de mesurer directement les paramètres de structure et vitesses de déplacement grâce à un système de digitalisation et d'analyse d'images.

Le cryostat est construit sur la base d'un cryostat MD 10 de Oxford Instruments, possédant une queue sur mesure avec fenêtres interchangeables. Le champ magnétique est produit par des anneaux de Helmholtz "normaux".

4. Performances optiques.

L'intérêt d'avoir une rotation plus grande du plan de polarisation sur les zones normales est double:

- il permet de gagner en contraste de manière évidente,
- mais surtout il nous offre la possibilité d'avoir des images beaucoup plus

lumineuses. Si nous supposons que:

- les zones superconductrices ne produisent aucune rotation,
- la rotation des zones normales vaut $\alpha = 2 \text{ V d H}_C$,

- le coefficient de transmission de l'optique vaut 0.01,
- le grossissement est d'environ 500 fois,
- les filtres polarisant ont un coefficient de transmission de 0.15 et d'extinction de 0.00015 soit un rapport d'extinction de plus de 10^{-5} ,

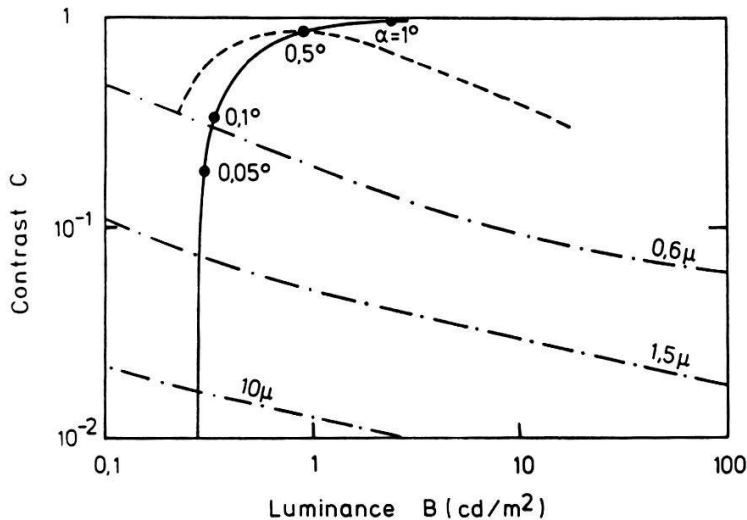


Figure 4.

Diagramme contraste-luminance.

- - - Limite de perception pour l'œil humain pour un grossissement de 500 fois,
- Contraste maximum pour différentes rotations,
- Contraste et luminance obtenus en faisant varier Θ .

le contraste entre une zone de luminance B et un fond de luminance B_0 est donné par:

$$C = \frac{B - B_0}{B_{\max}}$$

où $B_{\max}$ est la plus grande valeur entre B et B_0 .

L'expression du contraste d'une image magnéto-optique est donné par:

$$C = \frac{2 \alpha \sin \Theta - \alpha^2}{\sin^2 \Theta + 2 e}$$

ainsi le contraste maximum n'est pas à polariseurs croisés mais est donné par:

$$\Theta = 0.5 (\alpha \sqrt{(\quad)^2 + 8 e})$$

Laeng (6) avait déjà mis en évidence le gain que l'on peut représenter sur le graphique ci-contre.

5. Conclusions.

Le gain en rotation dû aux couches de selenure d'euprôm nous permet d'accéder à des domaines de contraste et donc de luminance beaucoup plus élevés, nous offrant la possibilité d'utiliser de nouveaux détecteurs tels que des caméras vidéo.

Entre autres personnes je remerciais Monsieur Schöpfer laborant pour son assiduité à la préparation des couches. Nos vifs remerciements également au Fond National pour son support financier.

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Total-energy electronic structure calculations for Fe₃Ni and FeNi.

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Abstract : We have performed total-energy calculations for ordered Fe-Ni compounds at different lattice constants using self-consistent non-magnetic (NM) and ferromagnetic (FM) LMTO energy band methods and local (spin) density formalism. Results are compared with experimental data and other calculations .

The electronic structure of FeNi alloys is a subject of considerable interest because these systems exhibit Invar anomalies such as instability of ferromagnetism, lattice softening and small thermal expansion coefficient at room temperature [1]. Williams et al. [2] analysed the volume dependence of the total energy for some ordered FeNi alloys providing some understanding of Invar systems. They showed that the total energy separation of the FM and NM state is very small near the Invar composition. In this work we try to pursue this type of study further by calculating properties related to the total energy with high precision. We perform accurate determination of total energies at different lattice constants for ordered fcc FeNi and Fe₃Ni compounds in both their NM and FM states using a self-consistent Linear Muffin-Tin Orbital (LMTO) band method [3,4] and local-spin-density (LSD) treatment of exchange and correlation [5]. Our self-consistent calculations do not use a Fixed-Spin-Moment (FSM) approach [6]. FSM has been advocated for calculations of magnetic systems which are near to instability since self-consistent convergence is made faster. However we have not used this procedure to achieve convergence since it is important to let the magnetic moment develop freely. Otherwise one may obtain the total energy for a magnetic configuration which is not at the variational minimum. The slow

convergence made it necessary to calculate band structure at a large number of k points (220 for Fe₃Ni and 396 for FeNi) in the irreducible Brillouin-zone (IBZ). The core states are not frozen but are recomputed during each self-consistent iteration. In addition the states were broadened with a 3 mRyd wide function. With this procedure we obtained a stable convergence of better than 1mRyd for the total energies. Other details of the calculations are similar as in ref. [7]. The calculated total energies were fitted to the Murnaghan's equation of state [8] with a rms error less than 10^{-6} Ryd/atom. The ground-state properties such as equilibrium lattice constant and bulk modulus are deduced from the fitting parameters and are compared with other calculations and with the experimental data in Table I.

Table I. Comparison of calculated lattice constant *a*, bulk modulus *B*, spontaneous magnetic moment *M* and experimental data.

		Non magnetic		Ferromagnetic			
		<i>a</i> (a.u)	<i>B</i> (Mbar)	<i>a</i> (a.u)	<i>B</i> (Mbar)	<i>M</i> (μ B/atom)	
						Fe	Ni
FeNi	other calculations						
	Williams et al. [2]	6.56	- - -	6.68	- - -	- -	- -
	Skriver et al. [9]	- - -	- - -	6.56	2.83	2.4	~0
	our calculation	6.50	3.29	6.60	1.97	2.36	0.5
	experiment [10]	- - -	1.92 (b)	6.765	1.77 (b)	2.6 (a)	0.7 (a)
Fe ₃ Ni	other calculations						
	Williams et al. [2]	6.54	- - -	6.68	- - -	2.00	0.5
	our calculation	6.48	3.04	6.57	1.60	1.65	0.4
	experiment [11]	- - -	1.77 (c)	6.761	1.08 (c)	1.1(d)	
	Fe ₇₀ Ni ₃₀						

(a) Values for disordered 50% FeNi alloy. (c) fcc 30%Ni FeNi alloy. (d) average moment

In figure 1 we show the total energy, the bulk modulus and the magnetic moment results as a function of lattice constant for the two compositions. The total energy difference ΔE between FM and NM state is very small (~ 0.5 mRyd/atom) for Fe₃Ni and is much larger ~ 7 mRyd/atom for FeNi. Clearly, in the former case, low-energy ($\Delta E \sim 80$ °K) thermal excitations would be sufficient to give the transition between the large volume FM state to the small volume NM state. In addition, the two states have different bulk moduli. Thus, qualitatively one can understand the Invar behaviour as a contraction of the atomic volume accompanied by a rapid

increase of the bulk modulus as the temperature increases. In FeNi ΔE corresponds to ~ 1000 °K, i.e. the necessary excitation for a transition is much larger or even not accessible. Another difference is that there is a rapid variation of the magnetic moments as a function of volume in Fe_3Ni but not for FeNi. This may reflect the small ΔE found in the Invar composition.

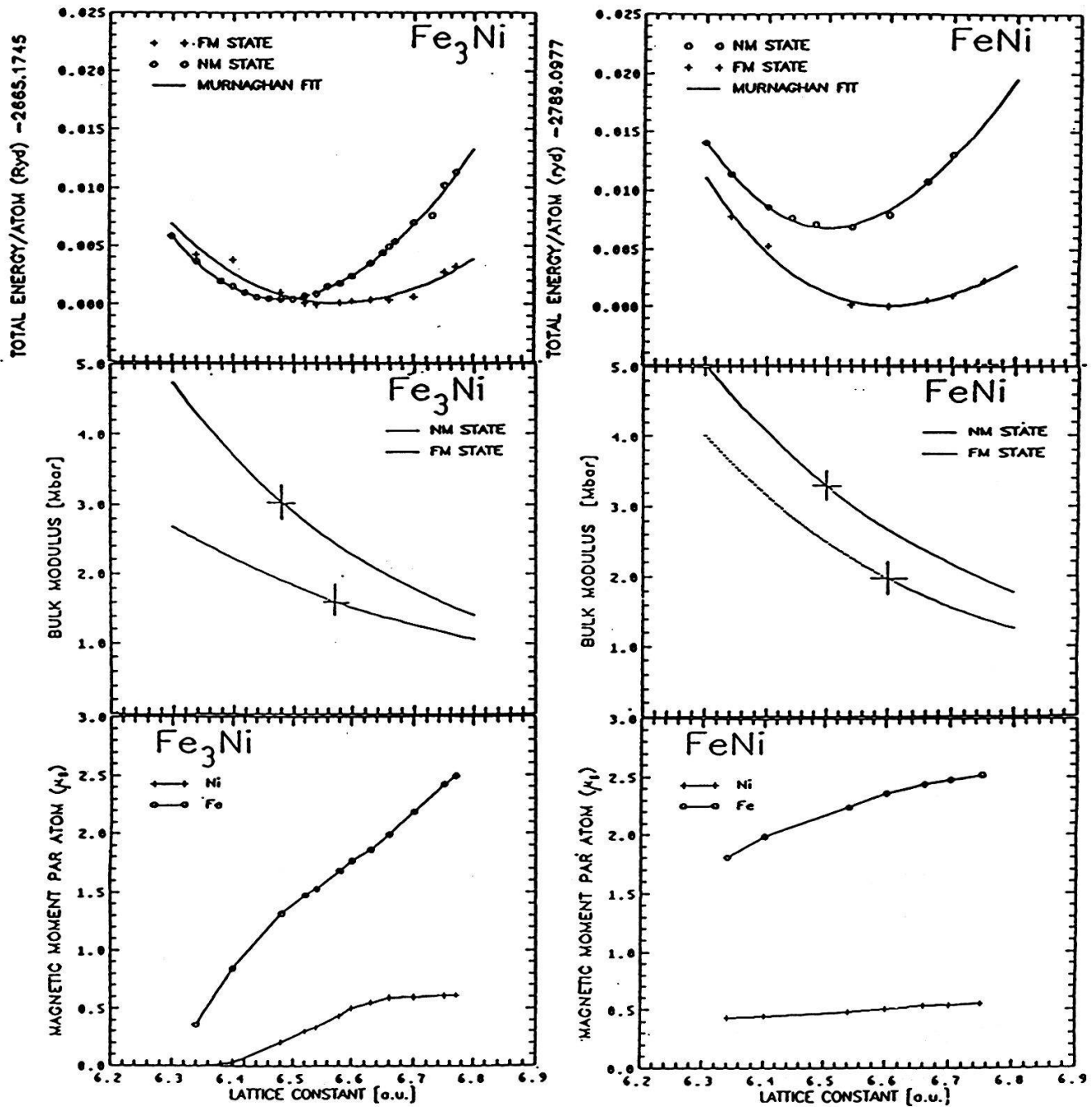


Fig. 1 : Total energy, bulk modulus and magnetic moment as a function of lattice constant.

Our results agree qualitatively with those of Williams et al. [2] although in details there are some differences. The positions of the total energy minima and their separation are somewhat shifted to smaller volumes and give smaller separations. In addition our calculations are sufficiently precise in order to derive values for the bulk modulus. At this stage we do not find that density of state (DOS) structures near the Fermi energy should be essential for Invar properties. In conclusion, we find that the small differences of total energy in FM and NM Fe₃Ni and large pressure variations of the magnetic moments are likely to be the origin of Invar behaviour.

Helpful discussions with G.P.Renaud, S.G.Steinemann and M.Peter are gratefully acknowledged.

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Optical and magneto-optical properties of NdS

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We report on measurements of the optical reflectivity between 0.03 and 12 eV and of the magneto-optical polar Kerr effect between 0.6 and 5 eV on NdS single crystals. In the Kerr effect structures are observed at 3 and 4.6 eV. The one at 4.6 eV is due to an $f \rightarrow d$ transition, while the peak near 3 eV has its origin in the particular values of the optical constants.

In the last decade great progress was made in the development of magneto-optical recording media. Among the most thoroughly investigated materials are amorphous alloys of the rare-earth elements Gd and Tb and the transition metals Fe and Co. The magneto-optical effects in these alloys are dominated by the transition metals since the magneto-optically active 4f - states of Gd and Tb are too far below the Fermi energy ϵ_F . In the case of $\text{Nd}_{1-x}\text{Co}_x$ films, on the other hand, Choe et al. [1] suggested that an appreciable contribution to the polar Kerr effect in the region of 4 eV is due to Nd. Ferromagnetic Nd_3S_4 also shows a pronounced structure in its $\tilde{\sigma}_{xy}$ spectrum in the same spectral range [2]. With the aim to confirm our presumption that these structures are due to a $4f^3 \rightarrow 4f^25d$ transition we performed optical and magneto-optical investigations on NdS. This metallic sulfide undergoes a transition from a paramagnetic to an antiferromagnetically ordered phase at $T_N = 9.3$ K. At the Néel temperature the cubic rocksalt structure of NdS distorts to a tetragonal structure in a distinct first-order transition [3].

All investigations have been made on cleaved (100) surfaces. The optical reflectivity between 0.03 and 12 eV was measured at room temperature only. In order to avoid birefringence as a result of the phase transition, the magneto-optical measurements in the range of 0.6 to 5 eV have been carried out above T_N at 15 K and in an external field of 100 kOe. Magnetic studies showed that even at 1.5 K the magnetization reaches only about $0.8 \mu_B/\text{Nd}$ in a field of 100 kOe, i.e. only a fraction on the free-ion value $3.27 \mu_B/\text{Nd}$. Our experimental set-up is described elsewhere [4].

As Fig. 1 indicates the optical reflectivity of NdS shows a behaviour typical for a metal. The steep decrease of the reflectivity between 2 and 3 eV, which is responsible for the golden colour of the compound, is as remarkable as the low value

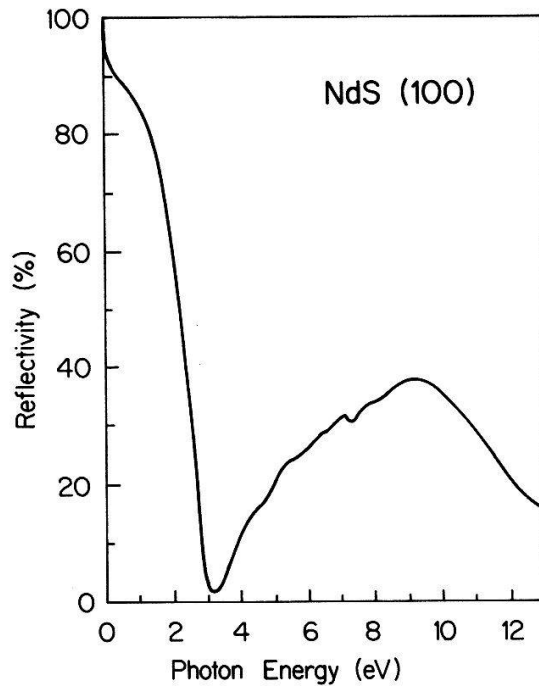


Fig.1: The near-normal-incidence optical reflectivity of NdS at room temperature.

of the minimum of 1.6 % at 3.2 eV. Above 3.5 eV the reflectivity shows a broad peak with a maximum of about 38 % at 9.3 eV.

From the reflectivity spectrum the optical conductivity σ_{1xx} , the energy loss function ζ , and the effective number of electrons n_{eff} contributing to optical transitions have been derived via the Kramers - Kronig transformation. The energy loss function $\zeta = \epsilon_2 / (\epsilon_1^2 + \epsilon_2^2)$ shows a strong peak at 2.75 eV, where $\epsilon_1 \approx 0$, $\partial\epsilon_1/\partial\omega > 0$ and ϵ_2 is small. This indicates a collective excitation, in this case a coupled plasmon. From a fit of $\sigma_{1xx} = \epsilon_2 \cdot \omega / 4\pi$ with a Drude ansatz one derives an unscreened plasma energy of $\hbar\omega_p = \hbar(4\pi Ne^2/m^*)^{1/2} = 5.5$ eV and a damping $\hbar\gamma = 0.33$ eV. Assuming one conduction electron per formula unit NdS we derive an effective mass $m^* = 0.98 m_e$. The pronounced structure between 4 and 10 eV can be assigned to $p(S) \rightarrow 5d(Nd)$ transitions in agreement with an increase of n_{eff} by $6 e^-$ /f.u. between 4 and 13 eV. One notices also a small shoulder just above 4 eV.

Fig . 2 shows the complex polar Kerr effect of NdS. In the neighborhood of the reflectivity minimum the rotation spectrum θ_K has its maximum of 3.54 deg at 3.12 eV and the ellipticity spectrum ϵ_K its minimum of -2.78 deg at 3.04 eV. In addition weak structures occur between 4 and 5 eV . The calculation of the real and imaginary parts of the off-diagonal conductivity (Fig. 3), however, leads to dominant structures around 4.6 eV, similar to those observed in Nd_3S_4 [2]. Based on this correspondence and the line shape we assign the structures around 4.6 eV to a $f \rightarrow d$ transition of Nd^{3+} .

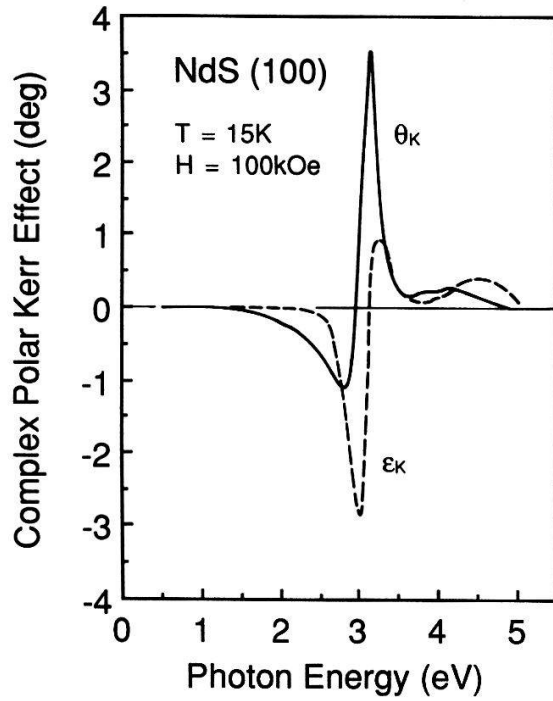


Fig. 2: The complex Kerr effect of NdS at 15 K and 100 kOe as a function of energy.

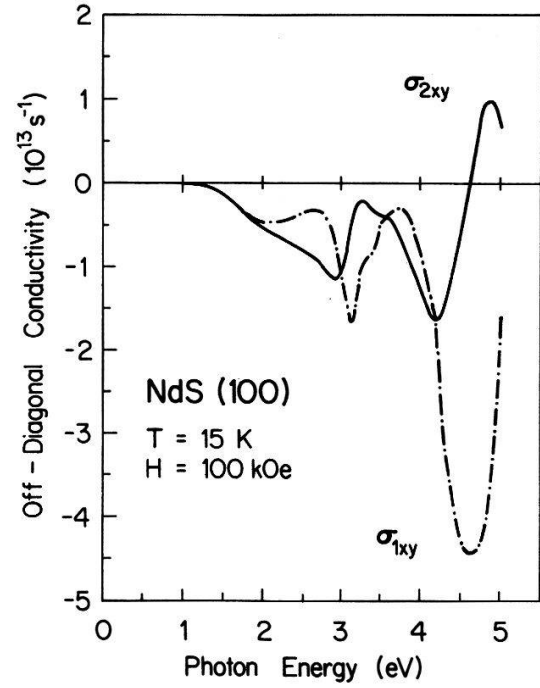


Fig. 3: The complex off-diagonal conductivity of NdS at 15 K and 100 kOe as calculated from the complex Kerr effect and the optical constants.

It is remarkable that, as in the case of Nd₃S₄, the strong peaks found in $\theta_K(\omega)$ and $\epsilon_K(\omega)$, are strongly suppressed in the $\tilde{\sigma}_{xy}$ spectra. This indicates that the Kerr rotation and ellipticity spectra of NdS near the plasma edge are dominated by the optical constants n and k . These enter into the expressions for

$$\theta_K = -(4\pi/\omega) [\{B/(A^2+B^2)\} \cdot \sigma_{1xy} + \{A/(A^2+B^2)\} \cdot \sigma_{2xy}] \quad (\text{eq. 1})$$

$$\epsilon_K = -(4\pi/\omega) [\{A/(A^2+B^2)\} \cdot \sigma_{1xy} + \{-B/(A^2+B^2)\} \cdot \sigma_{2xy}] \quad (\text{eq. 2})$$

via the coefficients $A = (n^3 - 3nk^2 - n)$ and $B = (-k^3 + 3nk^2 - k)$.

As an illustration Fig. 4 displays the prefactors $A/\omega(A^2+B^2)$ and $B/\omega(A^2+B^2)$ as a function of the photon energy for $T = 300$ K. At the moment it is not clear whether the remaining structures in $\tilde{\sigma}_{xy}$ near 3 eV are due to a change of the optical constants between room temperature and 15 K. Yet, this effect is rather small and

the dominant part of the signal in θ_K and ϵ_K near 3 eV has to be assigned to the resonance of the prefactors of σ_{1xy} and σ_{2xy} in eqs. (1) and (2).

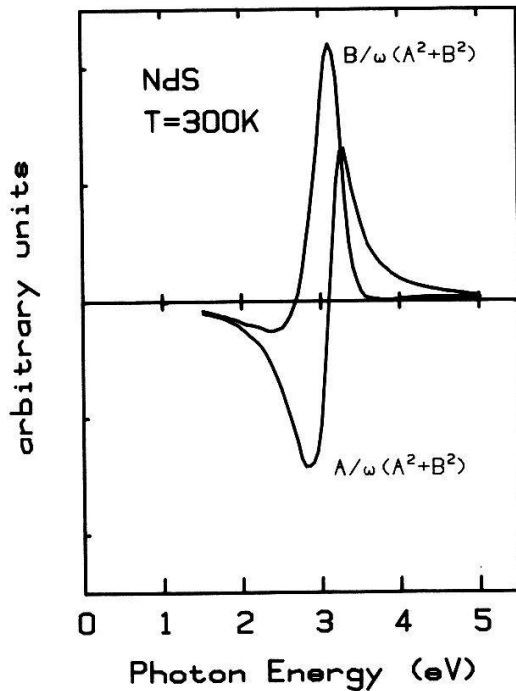


Fig 4: The prefactors $A/\omega(A^2+B^2)$ and $B/\omega(A^2+B^2)$ as a function of the photon energy for $T = 300$ K.

Thus, on the example of NdS, we have confirmed an earlier interpretation [2] that the $Nd^{3+} f \rightarrow d$ transition takes place near 4.5 eV. At the same time we have shown that optical constants can be responsible for the occurrence of a large magneto-optical effect.

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OPTICAL PROPERTIES OF EuMo_6S_8

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EuMo_6S_8 is an important compound for the understanding of magnetic superconductors. We report first reflectivity measurements in the energy range of 0.03 to 12 eV on EuMo_6S_8 and the interpretation of these data in the context of a band structure calculation. The real part of the optical conductivity is decomposed in two intraband and six interband contributions. The two intraband contributions can be assigned to electrons in the conduction band and holes in the valence band. Comparing this decomposition with the calculated joint density of states for $p(\text{S}) \leftrightarrow d(\text{Mo})$ transitions allows an assignment of five out of the six Lorentz oscillators. The sixth oscillator is at 1.7 eV and might be assigned to an $f^7(\text{Eu}) \rightarrow d(\text{Eu})$ transition.

During the last fifteen years extensive studies on the ternary rare earth compounds $(\text{RE})\text{Mo}_6\text{X}_8$ ($\text{X} = \text{Se}, \text{S}$) have been carried out and various interesting features resulting from the interaction between superconductivity and magnetism have been discovered [1]. The Chevrel phase EuMo_6S_8 was expected to be superconducting as well, because it is isoelectric and isostructural to PbMo_6S_8 and SnMo_6S_8 , which are good superconductors with $T_c \simeq 14$ K [2]. But a structural phase transition at 110 K from a room temperature rhombohedral to a low temperature triclinic structure suppresses superconductivity [3]. At pressures higher than 13 kbar, the structural phase instability vanishes and superconductivity appears. Despite the absence of a Meissner effect this pressure induced superconductivity is believed to be a bulk phenomenon [4].

In this work we report first room temperature measurements of the near normal incidence reflectivity on a polished polycrystalline sample of EuMo_6S_8 . The sample was synthesized at Geneva by Ø. Fischer and co-workers. The experimental set-up is described elsewhere [5]. Figure 1 shows the reflectivity spectrum in the energy range of 0.03 to 10 eV, as measured at room temperature and atmospheric pressure. For energies down to zero energy the reflectivity reaches 100 %, indicating a metallic behaviour. At higher energies some interband transitions are recognizable. To discuss these transitions and the free carrier behaviour, we calculate out of the reflectivity spectrum the real part σ_{1xx} of the optical conductivity using the Kramers-Kronig relation. This spectrum is shown in Figure 2. The low energy part (< 1 eV) is dominated by the free carrier contri-

bution, which produces the steep increase of σ_{1xx} towards zero energy. At higher energies, one can reveal several structures. In a simple atomic model, we tried to fit the main features of the spectrum with Lorentzian curves, yielding six oscillators for the interband transitions (labelled 1 to 6 in fig. 2) and two oscillators with zero resonance energy for the free carrier contribution. The fitted resonance energies, plasma energies and dampings are given in table 1. The error of these values is less than 0.05 eV, meaning, that with the given free parameters one gets the best agreement with the experimental curve within this error. Looking first at the two free carrier contributions, one can interpret them in a simple two band model as an electron contribution (oscillator a in table 1) originating from the Mo-4d conduction band, and a hole contribution (osc. b) from the S-3p valence band. The ratio of the square of the two unscreened plasma energies yields $(\hbar\omega_{pc}/\hbar\omega_{pv})^2 = 44$. This is equal to the ratio of the density of the free carriers $N(d)/N(p)$ times the ratio of the effective masses $m_v^*(p)/m_c^*(d)$. Supposing a value of $m_c^* = 0.5 m_e$ and $m_v^* = 3 m_e$, we get a ratio $N(d)/N(p) = 7.3$ in good agreement with the ratio of the density of states at the Fermi energy $D_d(\epsilon_F)/D_p(\epsilon_F)$ of a selfconsistent band structure calculation [6]. Such a two band model had been proposed for the low temperature phase to explain Hall measurements [7]. A ratio of

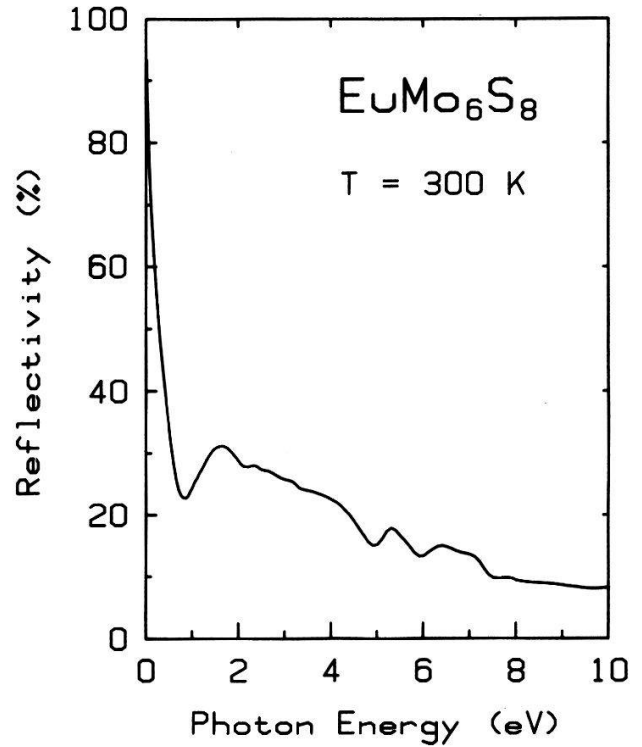


Fig. 1. The near normal reflectivity of EuMo_6S_8 at 300 K.

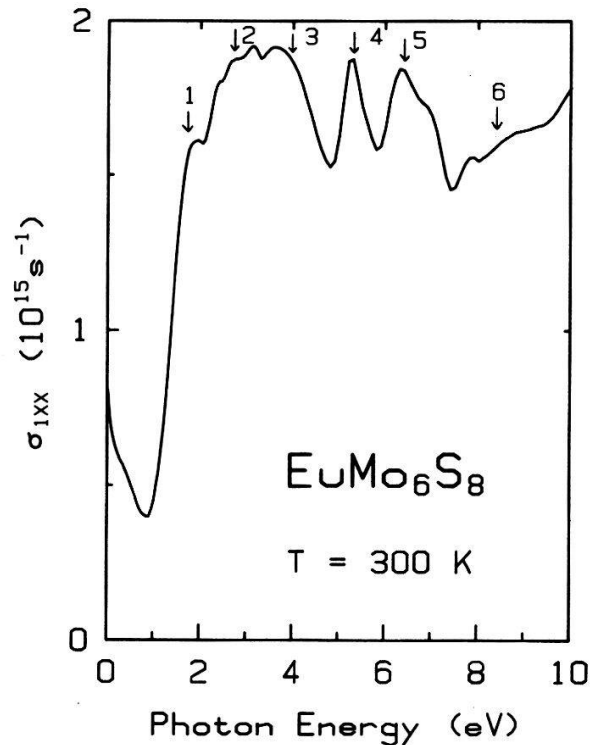


Fig. 2. The real part of the optical conductivity of EuMo_6S_8

osc.	$\hbar\omega_0$ (eV)	$\hbar\omega_p$ (eV)	γ (eV)	osc.	$\hbar\omega_0$ (eV)	$\hbar\omega_p$ (eV)	γ (eV)
1	1.70	2.50	0.80	5	6.40	2.70	1.00
2	2.70	4.40	1.80	6	8.30	5.60	4.00
3	3.95	4.25	2.00	a	0.00	1.98	0.75
4	5.30	2.15	0.75	b	0.00	0.30	0.08

Table 1. The parameters of the fitted Lorentz oscillators

the mobility $\mu_v/\mu_c = 0.5$ was suggested there. With our assumptions we get a ratio $\mu_v/\mu_c = 1.5$ for the room temperature phase.

To discuss the interband transitions, we calculate out of the band structure data, which was obtained in a self-consistent procedure, treating the Eu-f electrons as core levels [6], the joint density of states, taking the matrix element as a constant equal to one. Furthermore, we can calculate the real part $\sigma_{1xx}^{\text{theor}}$ of the optical conductivity. Figure 3 shows the theoretical total and partial $\sigma_{1xx}^{\text{theor}}$ spectrum. The low energy region up to 5 eV is dominated by $\text{Mo}_6\text{-d} \rightarrow \text{S-p}$ transitions, whereas the region above 5 eV consists mostly of $\text{S-p} \rightarrow \text{Mo}_6\text{-d}$ transitions. A comparison of the experimental with the theoretical σ_{1xx} is given in figure 4. The numbered arrows indicate the position of the six interband transitions, which were fitted to the experimental curve. For the discrepancy at high energies two main reasons can be listed: First, setting the matrix element equal to one is certainly a too restrictive simplification. Second, if one compares the effective number N_{eff} of electrons involved in the optical transitions for the theoretical and experimental data, the latter reaches 22 electrons per formula unit, whereas the theoretical calculation yields 30 electrons per f.u.. Because EuMo_6S_8 has in total 86 valence electrons, both values are rather low. The small experimental N_{eff} could be caused by scattering losses in the reflectivity at high energies, because our polycrystalline sample didn't have a very good surface. This leads for high energies to a too small value for σ_{1xx} . Looking at the peak positions of the six fitted interband transitions, one notices, that the theoretical $\sigma_{1xx}^{\text{theor}}$ exhibits distinct structures at the same energy as transition 2 to 6. Only for transition 1 at 1.7 eV there is no pronounced peak in $\sigma_{1xx}^{\text{theor}}$. Furthermore, $\sigma_{1xx}^{\text{exp}}$ is larger than $\sigma_{1xx}^{\text{theor}}$ around that energy. This could be a hint, that there is a transition not having been taken into account by the band structure calculation. Therefore we tentatively assign this transition at 1.7 eV to an $f^7(\text{Eu}) \rightarrow d(\text{Eu})$ transition. From the comparison with $\sigma_{1xx}^{\text{theor}}$, we can make a tentative assignment for the five remaining transitions, too. Number 2: $\text{Mo}_6\text{-d} \rightarrow \text{S}_2\text{-p}$,

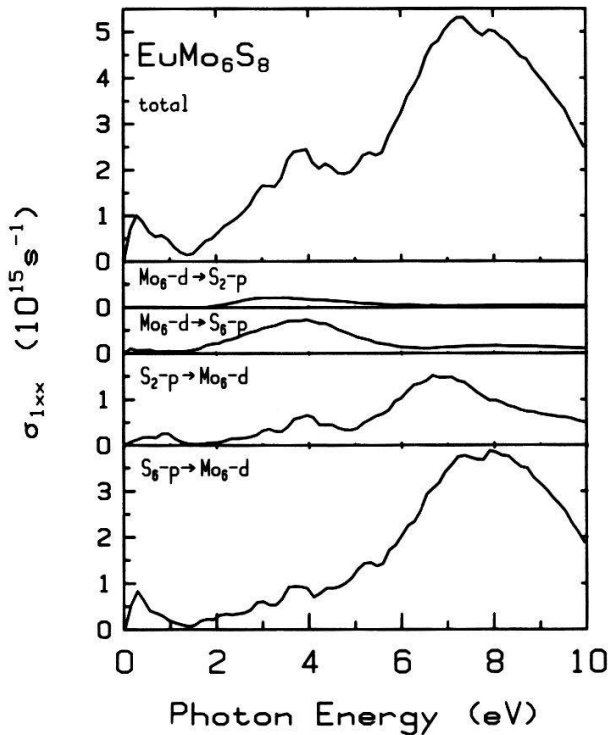


Fig. 3. The real part of the theoretical optical conductivity, as derived from a band structure calculation.

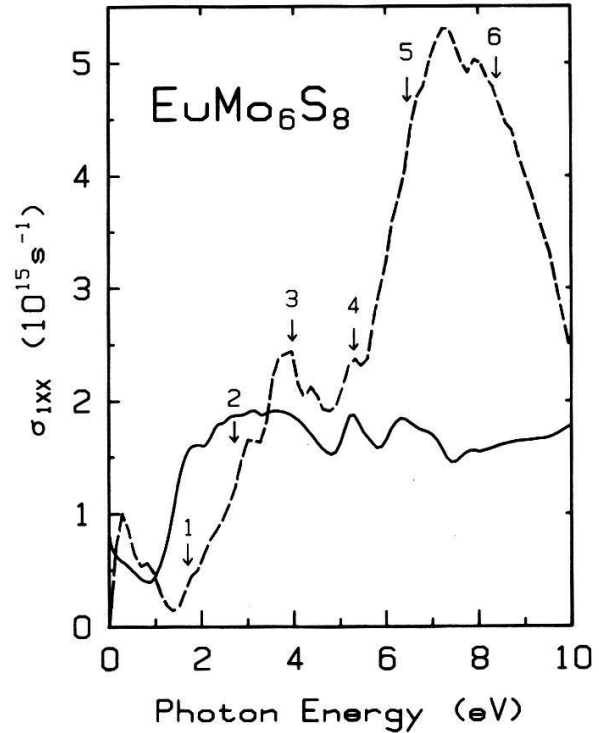


Fig. 4. The real part of the theoretical (broken line) and experimental (solid line) optical conductivity.

3: $\text{Mo}_6\text{-d} \rightarrow \text{S}_6\text{-p}$, 4: $\text{S}_6\text{-p} \rightarrow \text{Mo}_6\text{-d}$, 5: $\text{S}_2\text{-p} \rightarrow \text{Mo}_6\text{-d}$, 6: $\text{S}_6\text{-p} \rightarrow \text{Mo}_6\text{-d}$.

In conclusion, we want to point out that it is striking, how well the band structure calculation produces the same main features in $\sigma_{1xx}^{\text{theor}}$ as the measurement, except for one transition. To decide, what is the nature of this unresolved transition, we will make magneto-optical measurements, where we might see an effect of the Eu-f electrons.

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Hall effect and electrical resistivity of UCuP₂ single crystals

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We report on resistivity measurements between 2 and 1000 K and Hall effect measurements between 4 and 300 K for ferromagnetic UCuP₂.

The U-Cu-ternaries crystallize in a high symmetry. UCuP₂ crystallizes in a tetragonal system with space group I4/mmm while UCu₂P₂, for example, has a hexagonal structure with space group P $\bar{3}$ m1. The ordering temperature of UCuP₂ is 76 K and the magnetic moment amounts to 0.98 μ_B [1]. The measurements of the electrical resistivity were carried out on single crystalline samples using the ac van der Pauw method. The Hall effect was measured on the same samples in magnetic fields up to 100 kOe, which were generated by a split-coil superconducting magnet [2].

The resistivity perpendicular to the c-axis of UCuP₂ between 2 and 1000 K is shown in fig. 1. The residual resistivity ρ_0 is 52 $\mu\Omega\text{cm}$. In the magnetically ordered phase the electrical resistivity follows a T^2 law up to 10 K. The ordering temperature manifests itself as a pronounced knee in the resistivity curve. The inset in fig. 1 shows the derivative $\partial\rho/\partial T$. A sharp maximum occurs at 73 ± 1 K which is somewhat lower than the reported T_C of 76 K.

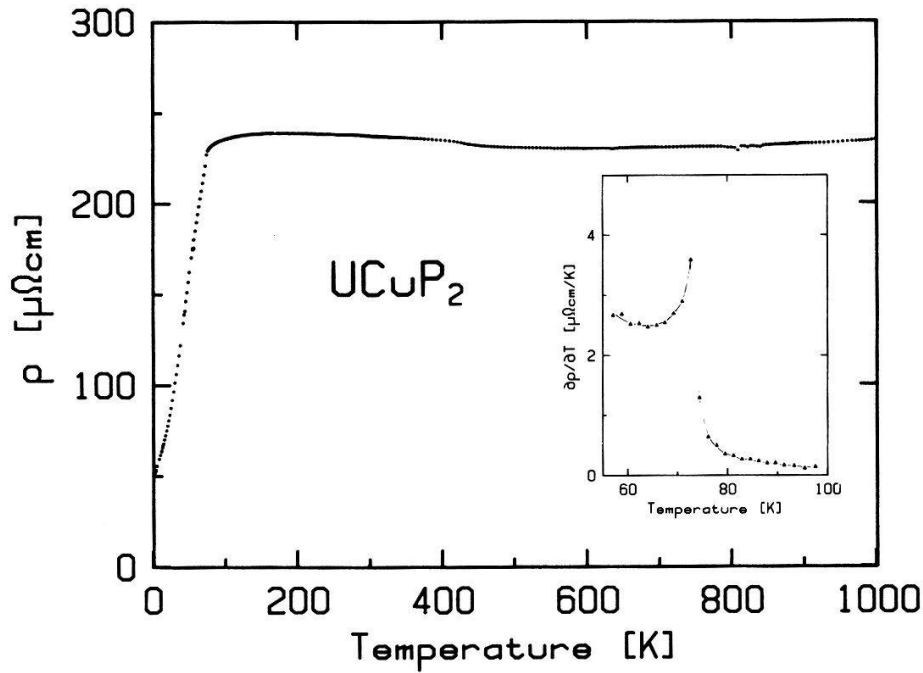


Fig. 1: Electrical resistivity in the a-b plane of UCuP_2 . The inset shows the derivative $\partial\rho/\partial T$.

Above T_C the resistivity decreases slightly up to about 400 K where it makes a little kink. From 400 up to 1000 K the resistivity curve goes through a very shallow minimum. This indicates that besides the linear phonon contribution there must be some other contribution with $\partial\rho/\partial T < 0$. A fit of the curve with the ansatz [3]:

$$\rho(T) = \rho_0 + c_{ph}T + c \ln(T) \quad (1)$$

gives the values $\rho_0 = 392.75 \mu\Omega\text{cm}$, $c_{ph} = 0.049 \mu\Omega\text{cm/K}$ and $c = -30 \mu\Omega\text{cm}$, suggesting the presence of a weak Kondo effect.

Fig. 2 displays the Hall resistivity of UCuP_2 in fields of 2 T and 4 T. The magnetic field is applied parallel to the c-axis, the current and voltage probes are in the isotropic a-b plane. We find a positive Hall effect with a maximum near 66 K. The empirical ansatz

$$\rho_H(B, T) = R_0(T)B + 4\pi M(B, T)R_S(T) \quad (2)$$

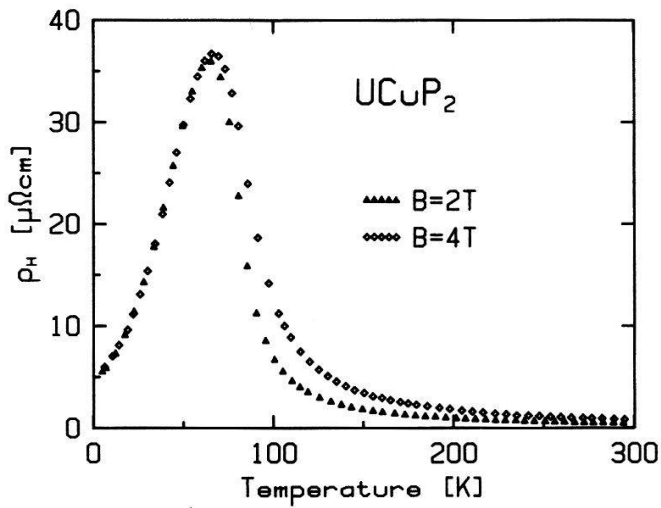


Fig. 2: Hall resistivity of UCuP_2 in fields of 2 and 4 T parallel to the c-axis.

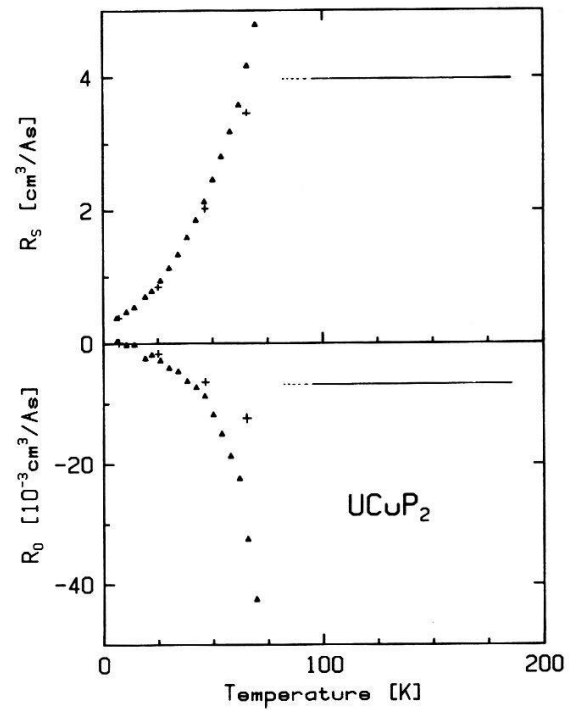


Fig. 3: Ordinary and extraordinary Hall coefficients R_0 and R_S of UCuP_2 (+) are determined from the field dependence of ρ_H at constant temperature, while (Δ) are calculated using the procedure described in the text. (—) shows R_0 and R_S in the paramagnetic region, were they are assumed to be constant.

provides for each temperature a system of two equations ($B = 2$ T and $B = 4$ T), which can be solved to separate R_H into the ordinary Hall coefficient R_0 and the extraordinary Hall coefficient R_S . Fig. 3 shows the results of such a decomposition for temperatures from 4 K to T_C , using magnetisation measurements on the very same sample in the same crystallographic direction.

In addition, we have performed for four different temperatures Hall measurements as function of magnetic fields up to 10 T. The crosses in fig. 3 show the corresponding values of R_0 and R_S which we have obtained using again eq. (2).

For $T > T_C$ R_0 and R_S are assumed to be constant. They can be determined by plotting $\rho_H(T)$ vs. $M(T)$. The values obtained are $R_0 = -6.7 \cdot 10^{-3} \text{ cm}^3/\text{As}$ and $R_S = 3.97 \text{ cm}^3/\text{As}$. If one uses the relation $R_0 = 1/ne$, which only holds for a single parabolic band, the value of R_0 corresponds to $n = 9.37 \cdot 10^{20}$ electrons per cm^3 or 0.063 electrons per formula unit ($e^-/\text{f.u.}$).

The parameter c of the Kondo term in (1) has been calculated with the formulas given in [3]. Choosing $J = 9/2$, $\epsilon_F = 1$ eV, $m^* = m$ the experimentally determined $c = -30 \mu\Omega\text{cm}$ gives $0.15 \text{ e}^-/\text{f.u.}$.

Both electron concentrations are very low compared to the low metallic resistivity indicating that the one-band model is inappropriate and that a multiple-band model should be applied for UCuP_2 . While in the conductivity the contribution of, for example, two bands are additive, in the Hall effect the two contributions depending on the sign of the carriers may have to be subtracted:

$$R_0 = (e/\sigma^2 c) (n_+ \mu_+^2 - n_- \mu_-^2) \quad (4)$$

This means that the total charge carrier concentration $n_+ + n_-$ is higher than n estimated from R_0 . The low electron concentration value derived from the Kondo term may then indicate that not all charge carriers are subject to Kondo scattering.

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INELASTIC LIGHT (RAMAN) SCATTERING FROM STRAINED ULTRA-SHORT SiGe SUPERLATTICES

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We have observed confined LO phonons in ultra-short period SiGe superlattices (SL's) grown on Ge(100) and $\text{Si}_{1-x}\text{Ge}_x(100)$. The confined LO phonons are shifted to lower energies compared to the bulk LO phonons of Si and Ge. The separation of the confinement and strain induced shifts follows from the known strain distribution and uniaxial stress parameters. Folded LA phonons confirm SL periodicities down to 8 monolayers.

Recently it has become possible to grow strained-layer SiGe superlattices (SL's) by the MBE-technique (1) despite of the rather large lattice mismatch of 4%. Depending on the underlying substrate (Si, Ge or $\text{Si}_{1-x}\text{Ge}_x$, respectively), the biaxial strain is either confined to the Ge-layers or the Si-layers or it can be shared by both with alternating sign.

We have investigated the lattice dynamics of the SL's by inelastic (Raman) light scattering. By considering the phonon dispersion of the constituent materials it can be concluded (2) that the phonons in the lower energy range ($0-200\text{cm}^{-1}$) are folded LA phonons of a material with the average composition of the SL, extending throughout the SL and experiencing the SL periodicity due to their long wavelength. The folded LA phonons can be described well by an elastic continuum model (3). The SL period is then determined by the observed energies of the folded LA phonons. Because of the reciprocal relationship of momentum space and real space the energy of the folded phonons depends more sensitively on the period d the smaller d is. This allows a very accurate determination of period d of ultra short SL's. Furthermore it can be seen (2), that the LO phonons lying at higher energies are sensitive to the microscopic structure of the specific layer type and are confined to one of the layers. For layer thicknesses in the range of a few monolayers the energies of these confined LO phonons are lowered with respect to the bulk phonons of Si and Ge (confinement effect). This lowering of the LO phonon energies through confinement is analogous to a particle with negative mass in an infinite potential well. In addition to the confinement shifts the LO

phonons shift to higher (lower) energies with biaxial compression (extension) of the layers. These strain-induced shifts of the LO phonons can be calculated from parameters obtained by uniaxial stress experiments (4). Knowing the lattice parameters from X-ray and Rutherford backscattering (RBS) measurements the strain within a specific layer is determined and a separation of strain and confinement induced shifts becomes possible.

The different neighboring atoms at the interfaces give rise to interface phonons. Due to similar covalent bonding their energy is mainly determined by the masses of the unlike atoms. Investigations of SiGe SL's on Si(100) has been given earlier (5,6). In this paper we consider SiGe SL's grown on thick (and hence relaxed) Ge and $\text{Si}_{1-x}\text{Ge}_x$ buffer layers on Si(100).

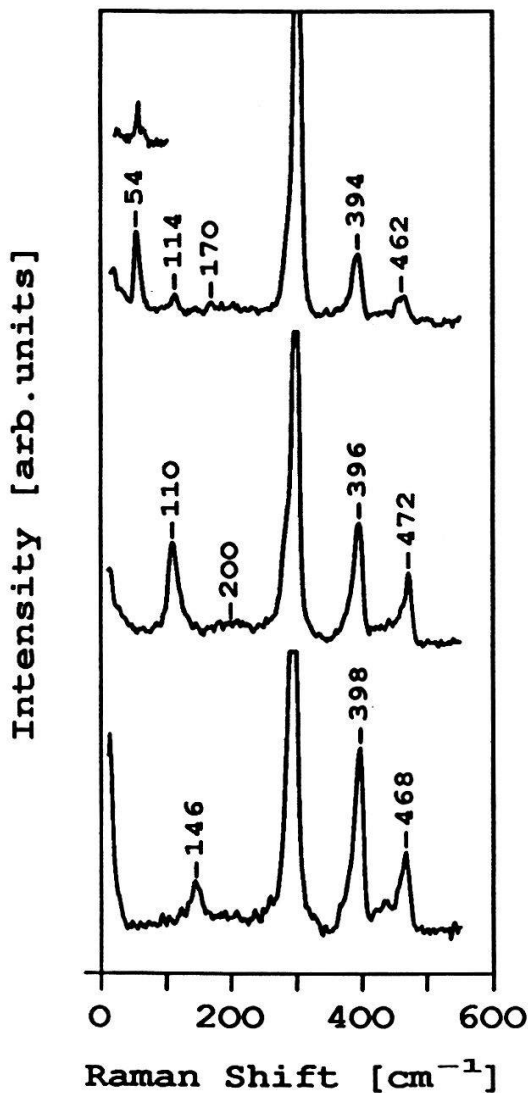


Fig. 1.

Raman spectra of three SiGe SL's on Ge(100) with different periods. (SL 256(top), 261, 257)

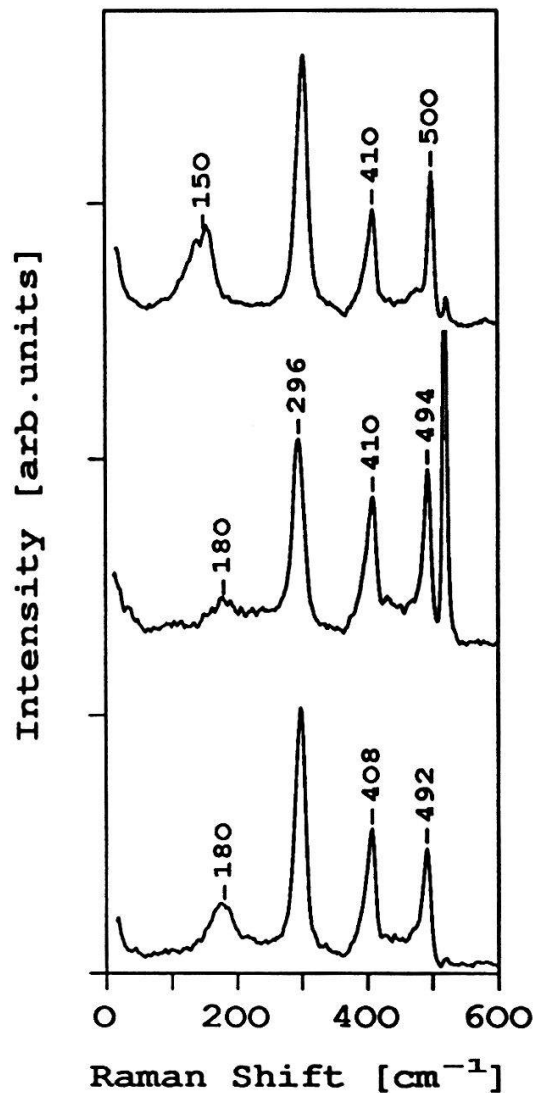


Fig. 2.

Raman spectra of three SiGe SL's on $\text{Si}_{0.5}\text{Ge}_{0.5}$ (100) with ultra-short periods. (SL 273(top), 275, 269)

The Raman experiments were performed in backscattering configuration with incident light polarized parallel to the (110) direction and with no analyzer in the scattered light beam. They were all carried out at room temperature in a helium atmosphere.

Fig. 1 shows the spectra of SiGe SL's grown on Ge(100) with three different periods. The first SL (256) with a period of 24 monolayers (ML's) shows folded phonons up to three orders. The first folded phonon doublet can be resolved. The confined Si-like LO phonon at 462 cm^{-1} is shifted downwards in energy by the striking amount of 60 cm^{-1} . The strain effect alone, due to the biaxial extension of the Si layers, calculates to a shift of 31 cm^{-1} . From the phonon dispersion of bulk Si a confinement induced shift of 25 cm^{-1} can be estimated for a 2.4 ML thick Si layer. The calculated strain and confinement effects thus explain the observed energy of the Si-like LO phonons. The second and third SL with periodicities of 12 ML (SL 261) and 9 ML (SL 257), respectively show a distinct first order phonon doublet. The SL period calculated from the energy of the folded phonons agrees well with the period obtained from X-ray measurements. The Si-like LO phonons in the two SL's are slightly less shifted in energy than in the first SL of fig. 1. The difference can be accounted for by the thicker Si layers and smaller confinement effect. These SL's show a Ge-like LO phonon at 298 cm^{-1} . The downward shift of 4 cm^{-1} from the bulk value is explained by an increasing confinement of the Ge-like phonons in comparison to SL 256. From the very similar bonding of Si and Ge, the different intensities of the confined LO phonons in the optical range ($250\text{--}550\text{ cm}^{-1}$) can be related to the relative thickness of the SL layers, if resonance can be excluded. The intensity of the interface phonons at $396\pm 2\text{ cm}^{-1}$ (fig. 1) relative to that of the confined LO phonons gives a qualitative measure of the interface structure (6).

Fig. 2 shows SiGe SL's grown on $\text{Si}_{0.5}\text{Ge}_{0.5}$ with different ultra short periods. The spectra of SL 273 with a period of 10 ML is seen in fig. 2 (top). It is surprising to see that the folded LO phonon doublet at 150 cm^{-1} is still resolved. The uncertainty of the period may therefore be less than one monolayer on the measured spot! It turns out that most of the other

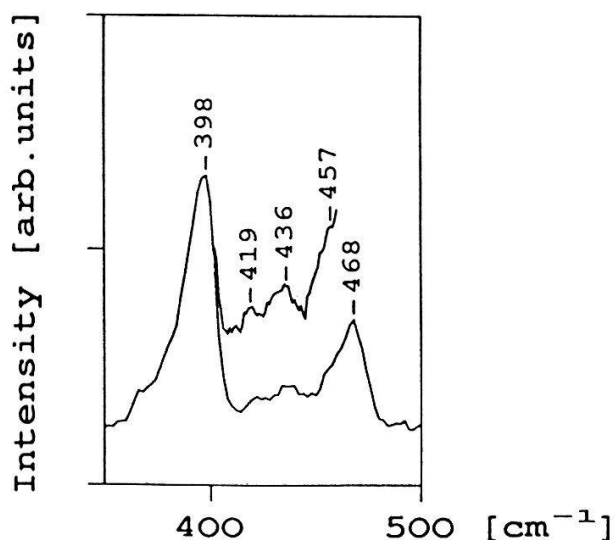


Fig. 3.

Raman spectra of SL 257 in the optic energy range.

spots on the sample do not show a resolved doublet, thus the period changes by about one ML across the wafer. X-ray and RBS measurements yield an average lattice constant and 1.7% and 2.3% strain in the Si and Ge layers respectively. We calculated for the Si-like LO phonons a stress induced shift of 13.2 cm^{-1} and a confinement induced shift of 10 cm^{-1} (4). The confinement and stress induced shift of the LO phonon in the compressed Ge layers cancel each other; the stress effect is opposed to the strain effect in this case. The two lower spectra of fig. 2 show SL's with a period of 8 ML and different overall thicknesses. The thinner of them shows a sharp peak at 522 cm^{-1} of the underlying bulk Si LO phonon of the substrate. This can also be weakly seen in the first spectrum. The folded phonon is now observed at 180 cm^{-1} and increases in intensity with the thickness of the SL. Note that the interface excitation lies at 410 cm^{-1} , which is considerably higher than in fig. 1 ($396 \pm 2 \text{ cm}^{-1}$). Its position is thus related to the strain in the neighboring layers as well. As a final remark we would like to point out that the structure seen between the interface peak and the Si-like confined LO phonon in fig. 1 becomes more pronounced in the spectra of the SL's with smaller periods. A more detailed peak structure is seen in fig. 3. Their interpretation in terms of modes analogous to slab modes and interface modes (7) and their relation to the electronic structure of the SL will be given elsewhere.

With inelastic light (Raman) scattering we observed confinement and strain effects in SL's of two different strain distributions in a number of samples down to ultra-short periods of 8 ML. A quantitative separation of confinement and strain effect has successfully been carried out. The elastic continuum model of folded LA phonons has been found to describe the folded LA phonons correctly even for SL's with a period of 8 ML's.

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LIGHT SCATTERING AT THE SOLID-LIQUID INTERFACE OF CYCLOHEXANE

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Abstract: Strong anomalous Rayleigh light scattering is observed on the liquid side of the crystal-melt interface of growing cyclohexane crystals. We measured the linewidth Γ and the intensity of the scattered light as a function of the scattering vector k and the polarization of the incident light. $\Gamma = D_1 k^2$ with $D_1 \sim 6 \cdot 10^{-9} \text{ cm}^2/\text{s}$. The angular intensity distributions exclude that the scattering originates from (diffusing) objects with smooth interfaces. The intensity distribution and its polarization dependence are compatible with a description of the interface layer by an Ornstein-Zernike pair correlation function.

1. Introduction

Anomalous Rayleigh scattering was first observed at the solid-liquid interface of water /1/ and then also in salol, cyclohexanol etc. /2,3,4/. For the first time we report the observation of the interface layer in a substance without permanent dipole moments. A model proposed by Cummins /5/ attributes the anomalous scattering to gaseous microbubbles. Dynamic light scattering data are compatible with that model, but not suitable to test it. Measurements of the intensity distribution and its polarization dependence are necessary for such a test.

2. Dynamic light scattering

The intensity autocorrelation function $g^{(2)}(\tau)$ can be fitted by a single exponential. For experimental details see /2/. The plot of Γ/k^2 in fig. 1 shows no departure of k^2 law. The dynamics can be described by a single diffusion constant $D_1 \sim 6 \cdot 10^{-9} \text{ cm}^2/\text{s}$. Using Stokes-Einstein relation this would correspond to a hydrodynamic radius $R_{\text{hyd}} \sim 0.26 \text{ }\mu\text{m}$.

3. Static light scattering or intensity measurements

The scattered intensity was measured for incoming polarization in the scattering plane ($i_{||}$) and normal to it ($i_{\perp}$). No significant depolarization was

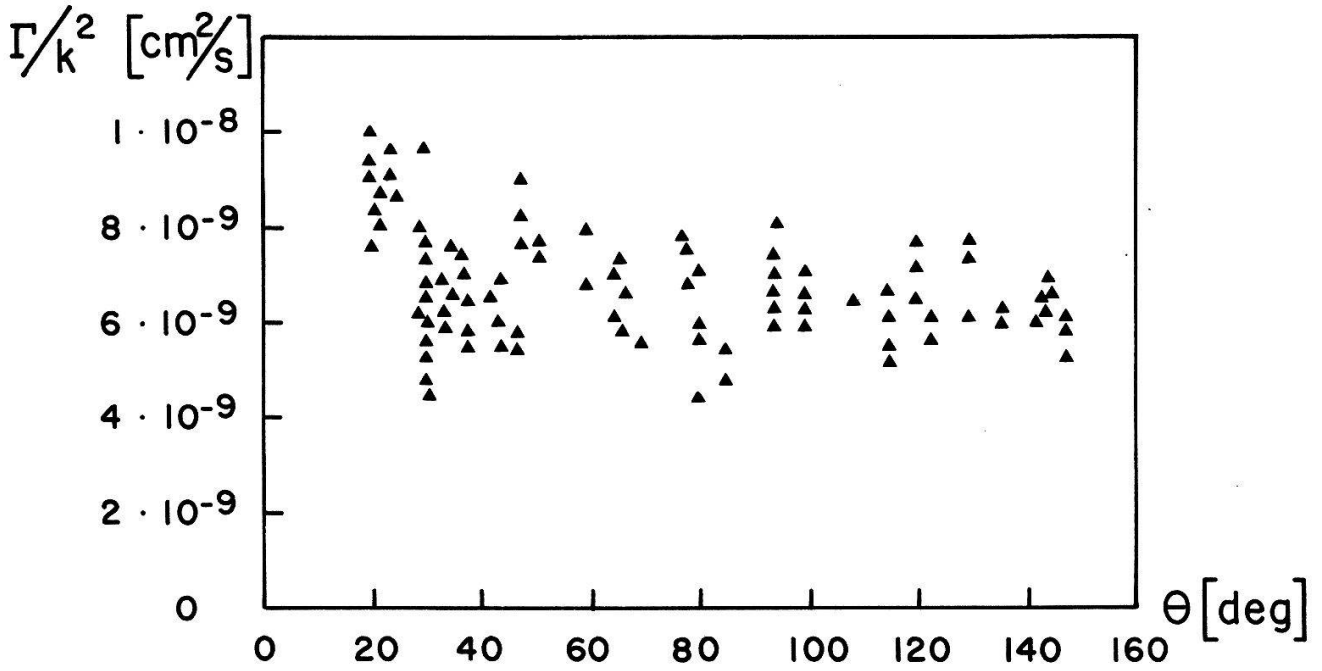


Fig. 1: $D_i = \Gamma/k^2$ vs. scattering angle Θ .

detected. In fig. 2a the scattered intensity is plotted as a function of the scattering angle Θ . We observe an increasing intensity with decreasing scattering angle. The deduction of the shape of the scattering objects from the angular anisotropy of the scattered intensity is generally not possible. Therefore we have calculated the intensity distribution for two models.

a) Homogeneous spherical particles: We calculated the diffraction pattern using Mie theory for various size parameters $\alpha = 2\pi r/\lambda$ and relative indice of refraction $m = n_{\text{sca}}/n_{\text{med}}$, where λ , n_{sca} , n_{med} and r are the wavelength of light in the medium, the index of refraction of the inhomogeneity, the index of refraction of the medium and the radius of the scatterers respectively. We used $1 \leq \alpha \leq 10$. $\alpha = 1$ leads to isotropic scattering and $\alpha = 10$ corresponds to $D_i = 3 \cdot 10^{-9} \text{ cm}^2/\text{s}$. Mie scattering curves usually show typical oscillations originating in the spherical symmetry of the particles. These oscillations are removed by allowing for a slight size distribution around α in our calculations. Independent of the choice of m , we found no α which fitted our data. All the calculated curves show negativ curvature for small angles (fig. 2b).

With a large size distribution of the form $N(\alpha) \sim \alpha^{-5}$; $1 < \alpha < 10$ the intensity distribution could be fitted, but the correlation function $g^{(2)}(\tau)$ would then no longer be exponential and the fitted linewidth would show a strong departure from k^2 law. Both are not observed.

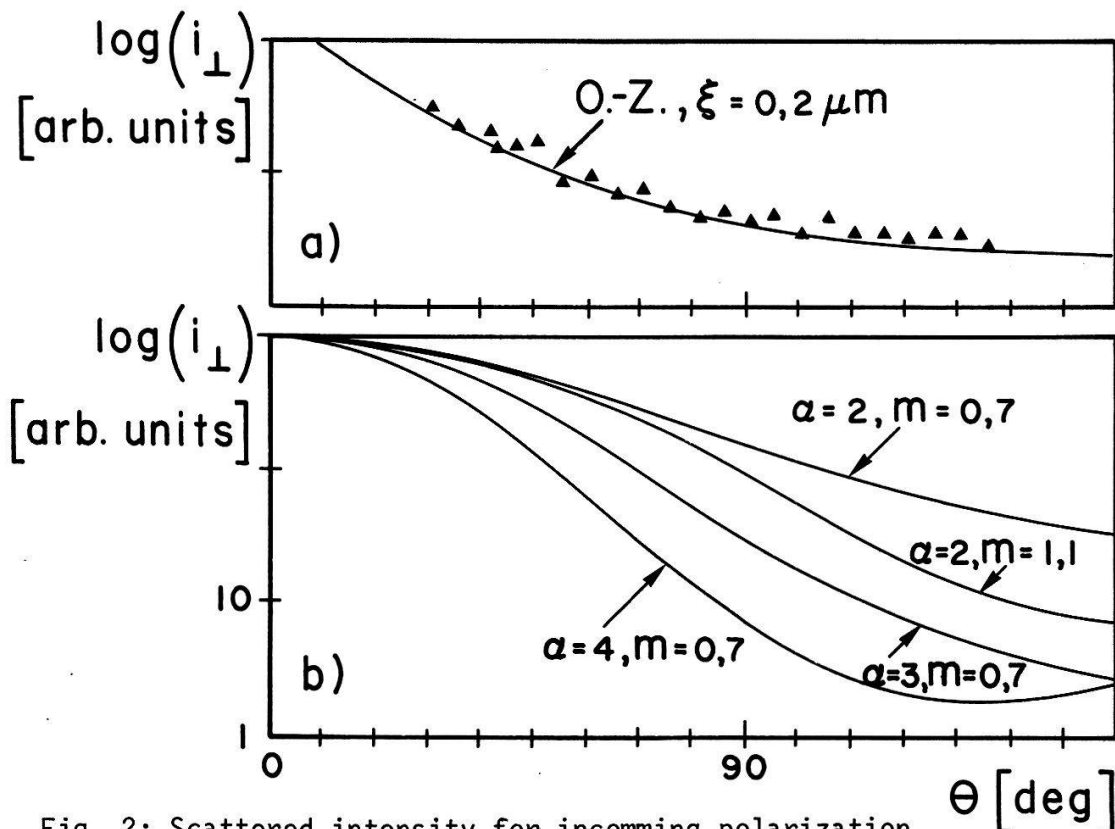


Fig. 2: Scattered intensity for incoming polarization normal to the scattering plane vs. scattering angle θ .

a: Experimental data ($\lambda=488$ nm). Drawn line corresponds to the Ornstein-Zernike function for $\xi=0.2 \mu\text{m}$ ($\lambda=488$ nm).

b: Calculated Mie diffraction patterns for various α and m .

b) Scattering by fluctuations: In an alternative treatment the medium can be described by a pair correlation function $\gamma(r)$. The scattered intensity is then given by the Fourier transform of $\gamma(r)$. The intensity data can be fitted by the Ornstein-Zernike form: $\gamma(r) \sim \frac{1}{r} \cdot e^{-r/\xi}$; $I(k) \sim (1 - k^2 \xi^2)^{-1}$, with $\xi \sim 0.2 \mu\text{m}$ (fig. 2a). This correlation length agrees with the one calculated from D_1 . Another correlation function $\gamma(r) \sim e^{-r/\xi}$ used by Debye and Bueche for inhomogeneities in lucite [6] can also account for the intensity profile. In that case the correlation length would be $\xi \sim 0.05 \mu\text{m}$.

Polarization

The ratio $i_{\perp}/i_{\parallel}$ of the scattered intensity in fig. 3. shows the usual Rayleigh positive polarization maximum at $\theta=90^\circ$. These data are compatible with model b). The model calculations for gas bubbles with $2.5 < \alpha < 7$ show: i) a broadening of the peak, ii) a decrease of $i_{\perp}/i_{\parallel}$ and iii) a shift of the maximum. This gives additional independent arguments against the gas bubbles model.

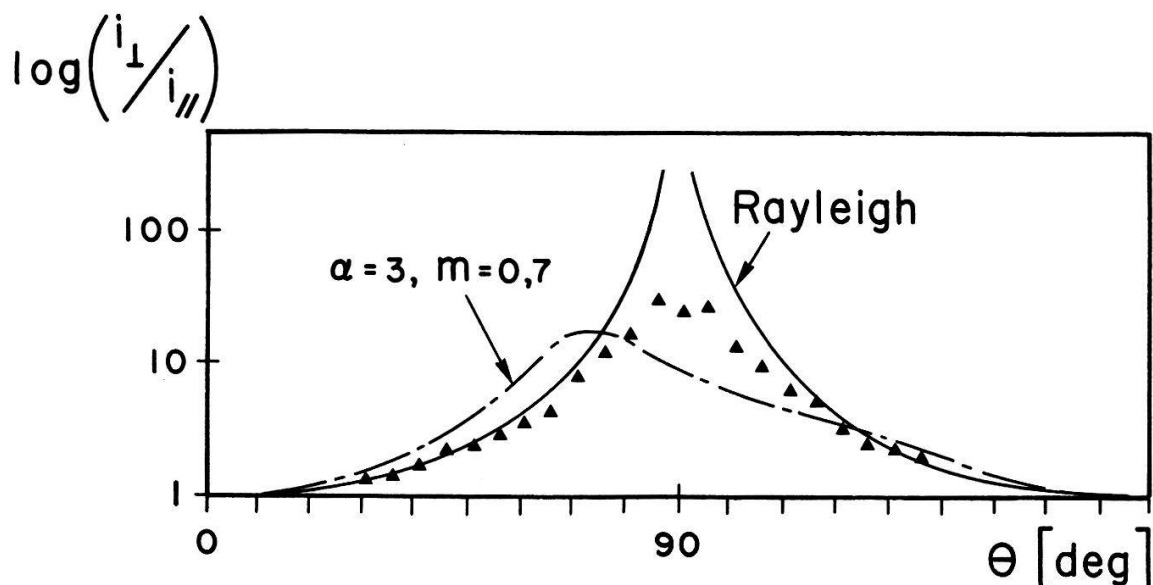


Fig. 3: Ratio $i_{\perp}/i_{\parallel}$ of the scattered intensity vs. scattering angle θ .

▲ Experimental data ($\lambda=488$ nm).

---- Rayleigh curve is given by $i_{\perp}/i_{\parallel}=1/\cos^2\theta$.

--- Mie calculation for gas bubbles.

4. Conclusions

We showed that the anomalous scattering at the crystal-melt interface of cyclohexane cannot originate from homogeneous particles moving in the liquid. A correct intensity distribution can be given e.g. by the Ornstein-Zernike or the Debye-Bueche correlation function. Our experiments with cyclohexane give evidence that density fluctuations at the solid-liquid interface are a general phenomenon of the freezing transition of dielectric materials.

This work was supported by the Swiss National Science Foundation.

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SCHWERE-KAPILLAR-WELLEN KLEINER AMPLITUDEN
UEBER SUPRAFLUIDEM HELIUM II

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Durch die Aussendung von Zweitem Schall in Helium II können auf der Oberfläche der Flüssigkeit Schwere-Kapillar-Wellen generiert werden [1].

Die Lagrange-Formulierung der Zweite Schallausbreitung in einem unendlich ausgedehnten Medium hat W. Lukosz eingeführt [2]. Jetzt wird eine entsprechende Behandlung spezifisch für das Oberflächenproblem vorgestellt (Fig. 1).

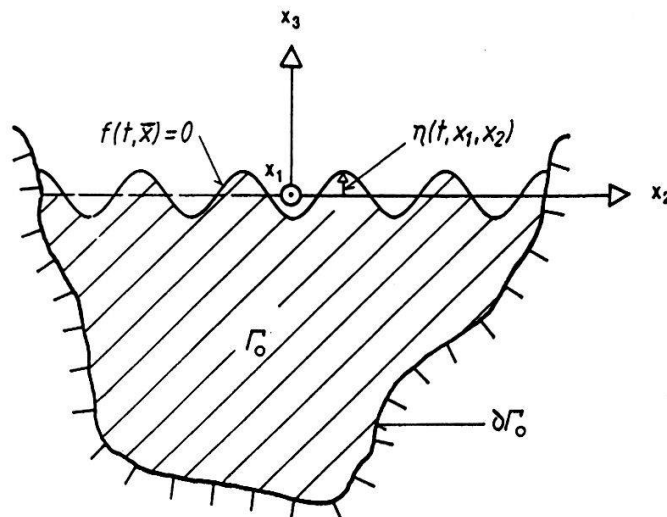


Fig. 1 - Querschnitt Γ_0 des Flüssigkeitsgebiets Γ mit freiem oberem Rand: $\eta = f + x_3$

Das Verhalten von Helium II wird im Zweifluidmodell durch zwei unabhängige Geschwindigkeits-Vektorfelder beschrieben. In unserem Modell wird vorausgesetzt der normale Anteil verhalte sich nebst dem suprafluiden auch rotationsfrei. So ist es zunächst sinnvoll eine Lagrangedichtefunktion, die im wesentlichen durch zwei Geschwindigkeitspotentiale bestimmt ist zu betrachten:

$$\varepsilon = \varepsilon(\Phi, \Phi_t, \Phi_{x_i}; p), \quad \Phi = (\phi_1, \phi_2), \quad i \in \{1, 2, 3\}. \quad (1)$$

Der Buchstabe p bezeichnet ein externes Druckfeld.

Mit dieser Lagrangedichtefunktion wird ein Wirkungsfunktional gebildet:

$$S = \int_{\Gamma} \int_{t_0}^{t_1} \mathcal{E}(\Phi, \Phi_t, \Phi_{x_i}; p) dt dV \quad (2)$$

Die Variation der Geschwindigkeitspotentiale liefert die Euler-Lagrange Gleichungen

$$\frac{\partial \mathcal{E}}{\partial \phi_{\alpha}} - \frac{\partial}{\partial t} \frac{\partial \mathcal{E}}{\partial \phi_{\alpha t}} - \frac{\partial}{\partial x_i} \frac{\partial \mathcal{E}}{\partial \phi_{\alpha x_i}} = 0 \quad \alpha \in \{1, 2\} \quad , \quad (3)$$

Randbedingungen für den festen Rand (der Kürze halber weggelassen) und die bewegliche Oberfläche:

$$\left. \frac{\partial \mathcal{E}}{\partial \phi_{\alpha t}} \right|_{\eta} \frac{\partial \eta}{\partial t} + \left. \frac{\partial \mathcal{E}}{\partial \phi_{\alpha x_1}} \right|_{\eta} \frac{\partial \eta}{\partial x_1} + \left. \frac{\partial \mathcal{E}}{\partial \phi_{\alpha x_2}} \right|_{\eta} \frac{\partial \eta}{\partial x_2} - \left. \frac{\partial \mathcal{E}}{\partial \phi_{\alpha x_3}} \right|_{\eta} = 0 \quad (4)$$

Es entsteht noch eine Gleichung, die von der Variation des Gebiets herrührt:

$$\mathcal{E} \Big|_{\eta} = 0 \quad (5)$$

Als nützlich erweist es sich die Lagrangedichtefunktion $\mathcal{E}$ nach $y_k \in \{t, x_1, x_2, x_3\}$ zu differenzieren und die Euler-Lagrange Gleichung (3) mit $\alpha = 1$ für eine Umformung zu benutzen. Setzt man anschliessend $y_k = x_i$, so kann durch Vergleich mit einer Formel, die aus den Gleichungen des Zweifluidmodells [3] folgt, die Lagrangedichtefunktion ermittelt werden:

$$\mathcal{E} = \rho_1 \frac{\partial \phi_1}{\partial t} - \frac{1}{2} \rho_1 \left(\frac{\partial \phi_1}{\partial x_k} \frac{\partial \phi_1}{\partial x_k} \right) + \frac{1}{2} \rho_2 \tilde{\lambda}_2 \phi_2^2 - \frac{1}{2} \rho_2 \left(\frac{\partial \phi_2}{\partial x_k} \frac{\partial \phi_2}{\partial x_k} \right) - p \quad (6)$$

$$\tilde{\lambda}_2 = \left(\frac{\omega_2}{c_2} \right)^2 \quad ; \quad \vec{v}_{\alpha} = - \vec{\nabla} \phi_{\alpha} \quad , \quad \alpha \in \{1, 2, n\}$$

ω_2 ist die Kreisfrequenz und c_2 die Schallgeschwindigkeit der Zweite Schallwellen. Es wurden die Bezeichnungen

$$\rho_1 = \rho \quad , \quad \rho_2 = \left(\frac{\rho_n}{\rho_s} \right) \rho_1 \quad , \quad \vec{v}_1 = \vec{v} \quad , \quad \vec{v}_2 = \vec{v}_n - \vec{v}_1 \quad (7)$$

eingeführt. ρ_n beschreibt den normalen und ρ_s den suprafluiden Massenanteil, wobei die Gleichung $\rho = \rho_n + \rho_s$ diese beiden mit der Dichte des Fluids verbindet. Die vorteilhafte Einführung des Vektorfeldes $\vec{v}_2$ geht auf F. London zurück [4] und enthält das Geschwindigkeits-Vektorfeld $\vec{v}_n$ der normalen Komponente.

Wird die Gleichung (6) in jene mit den Nummern (3) und (4) eingesetzt, so erhält man:

$$\Delta \phi_1 = 0 \quad (7/1)$$

$$\left. \frac{\partial \eta}{\partial t} - \frac{\partial \phi_1}{\partial x_1} \right|_{\eta} \left. \frac{\partial \eta}{\partial x_1} - \frac{\partial \phi_1}{\partial x_2} \right|_{\eta} \left. \frac{\partial \eta}{\partial x_2} + \frac{\partial \phi_1}{\partial x_3} \right|_{\eta} = 0 \quad (7/2)$$

Die erste Gleichung ist die Laplace Gleichung und beschreibt Potentialströmungen. Die zweite heisst kinematische Randbedingung und tritt auch bei der Beschreibung gewöhnlicher Flüssigkeiten auf [5].

$$\Delta \phi_2 + \tilde{\lambda}_2 \phi_2 = 0 \quad (8/1)$$

$$\left. \frac{\partial \phi_2}{\partial x_1} \right|_{\eta} \left. \frac{\partial \eta}{\partial x_1} + \frac{\partial \phi_2}{\partial x_2} \right|_{\eta} \left. \frac{\partial \eta}{\partial x_2} - \frac{\partial \phi_2}{\partial x_3} \right|_{\eta} = 0 \quad (8/2)$$

Mit $\phi_2 = \phi_n - \phi_1$ und (7/2) folgt sofort:

$$\left. \frac{\partial \eta}{\partial t} - \frac{\partial \phi_n}{\partial x_1} \right|_{\eta} \left. \frac{\partial \eta}{\partial x_1} - \frac{\partial \phi_n}{\partial x_2} \right|_{\eta} \left. \frac{\partial \eta}{\partial x_2} + \frac{\partial \phi_n}{\partial x_3} \right|_{\eta} = 0 \quad (8/3)$$

Es werden nur Massen- (7/2) und Entropieanteile (8/3), die tangential zur (bewegten) Oberfläche transportiert werden in dieser Theorie berücksichtigt; die Verdampfung von Helium II wird ausgeschlossen.

Für kleine Heizleistungen und Amplituden der Oberflächenwellen können die Systeme (7) und (8) -die durch die dynamische Randbedingung (5)/(6) gekoppelt sind- linearisiert und analytisch gelöst werden:

$$\eta(t, x_1) = \tilde{\eta} \frac{c_g^2}{c_g^2 + c_c^2} \left[1 + \frac{c_g^2 + c_c^2}{c_c^2 - (c_g^2 + c_c^2)} \cos(2\omega_2 t) \right] \cos(2k_2 x_1) \quad (9)$$

Im Resultat (9) des zweidimensionalen Modells, in dem periodische Randbedingungen und eine unendliche Flüssigkeitstiefe vorausgesetzt werden, bezeichnet c_g die Phasengeschwindigkeit reiner Schwere- und c_c jene reiner Kapillarwellen.

$$\tilde{\eta} = \frac{1}{4g} \left(\frac{\rho_2}{\rho_1} \right) k_2^2 (\tilde{\phi}_2)^2 \quad (10)$$

$\tilde{\phi}_2$: Amplitude des Geschwindigkeitspotentials ϕ_2 .

Sorbello [6] hat zum vornherein Massenfluss ausgeschlossen und daher nur die Lösung des Spezialfalls (3) erhalten (Fig. 2).

Diese wurde von ihm als zeitlicher Mittelwert $\langle \eta \rangle$ der Oberflächenauslenkung interpretiert. Die durchgeführten Berechnungen beweisen jedoch, dass für den experimentell untersuchten Frequenzbereich ($1000 \text{ Hz} < f_2 < 10'000 \text{ Hz}$) [1], die apriorische Voraussetzung $\vec{v}_1 \equiv 0$ auch bei einer Untersuchung momentaner Oberflächenprofile standhält. Zudem wird gezeigt, dass beim Uebergang zu tieferen Frequenzen He II-Oberflächen - durch langsamere Druckschwankungen angeregt-erzwungene Schwingungen auszuführen beginnen.

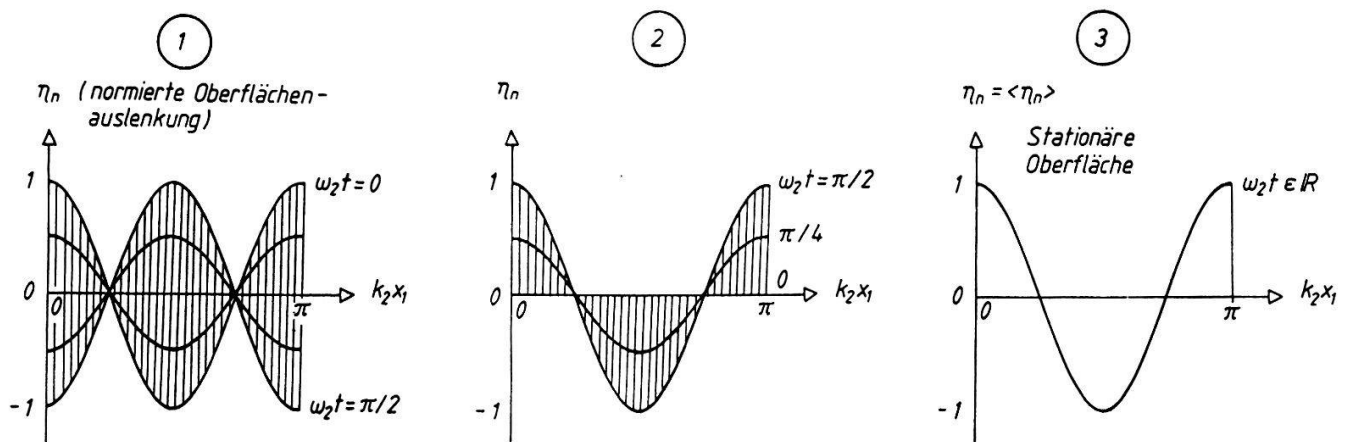


Fig. 2 - Verhalten der Oberfläche von He II unter periodischen Störungen verschiedener Frequenzen.

Dank gebührt Prof. Dr. J.L. Olsen.

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**BOMBARDEMENT IONIQUE AVEC DES IONS D'IODE:
EFFETS EN SURFACE**

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Abstract: Ion milling is one of the techniques used to obtain thin films for the high resolution transmission electron microscopy (HREM). The iodine ion milling has been used to thin some GaAs crystal with two different energies of the ions; an amorphous layer is still created at the crystal surface. A slightly higher surface roughness is resulting from the iodine ion milling.

1. Introduction

La microscopie électronique à haute résolution en transmission (HREM) permet d'observer les structures jusqu'au niveau des distances interatomiques. Quelle que soit la technique de préparation utilisée, seules des lames minces libres de défauts sont interprétables. Il faut d'une part qu'il y ait le moins possible de dégâts à l'intérieur du cristal dus aux impacts des ions incidents, et d'autre part que la couche amorphe en surface soit la plus mince possible. La surface du cristal doit présenter le moins possible de marches, c'est-à-dire que la rugosité de celle-ci doit être la plus faible possible.

2. Méthodes et résultats

Dans un précédent article⁽¹⁾, l'épaisseur de la couche amorphe en surface de GaAs a été étudiée dans le cas du bombardement avec des ions d'argon en utilisant la technique de la coupe transverse. L'étude a été poursuivie avec des ions d'iode qui semblent plus appropriés pour les semiconducteurs^(2,3) en raison de leur masse élevée et de leur caractère réactif. L'effet des ions d'iode de 2keV et 5keV sur un échantillon à température ambiante a été observé. L'attaque se fait pendant une heure, sous un angle de 20° et avec un échantillon tournant. Les résultats sont comparés aux meilleures conditions pour l'argon (ions de 2keV avec un échantillon à la température de l'azote liquide). La comparaison sera faite du point de vue de la rugosité de la surface ainsi obtenue et de la qualité du cristal jusqu'à la zone amorphe de surface.

Pour limiter les dégats introduits dans la deuxième phase de la préparation, c'est-à-dire l'amincissement de la coupe transverse, les meilleures conditions ont toujours été utilisées (ions d'argon à 2keV et échantillon refroidi à l'azote liquide).

Après le bombardement avec l'iode, le profil de la région attaquée des deux conditions a été mesuré à l'aide d'un rugosimètre TENCOR par contact d'un stylet sur la surface.

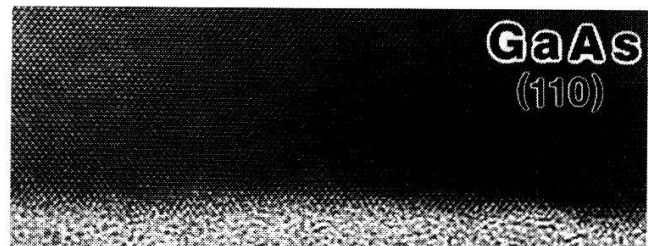
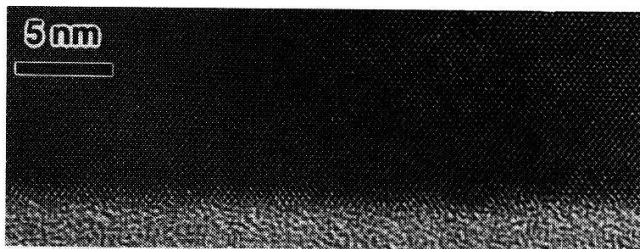


Figure 1.: 2 clichés HREM d'un échantillon de GaAs préparé avec des ions d'argon de 2keV d'énergie et placé à la température de l'azote liquide.

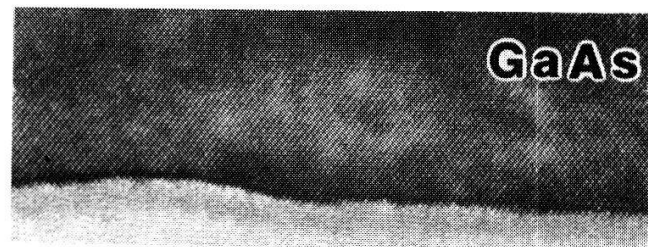
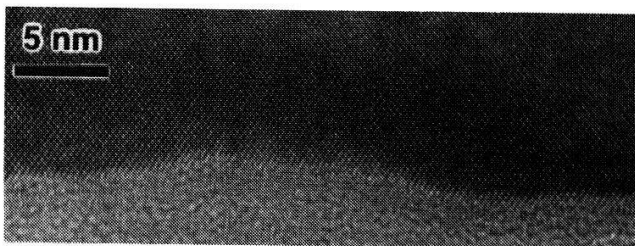


Figure 2.: GaAs préparé avec des ions d'iode de 5keV d'énergie.

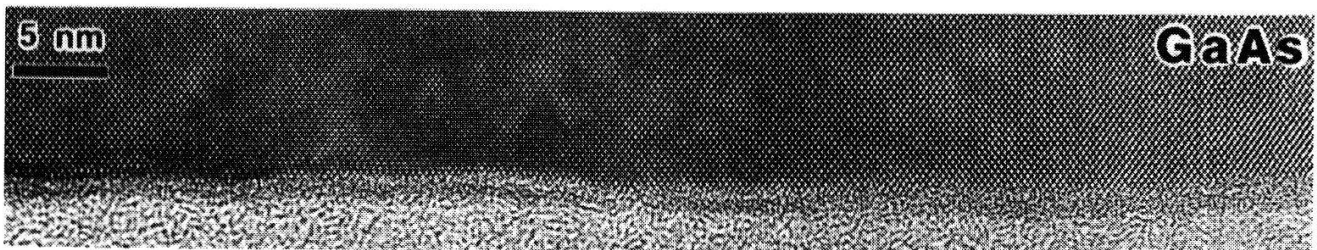


Figure 4.: GaAs préparé avec des ions d'iode de 2keV d'énergie.

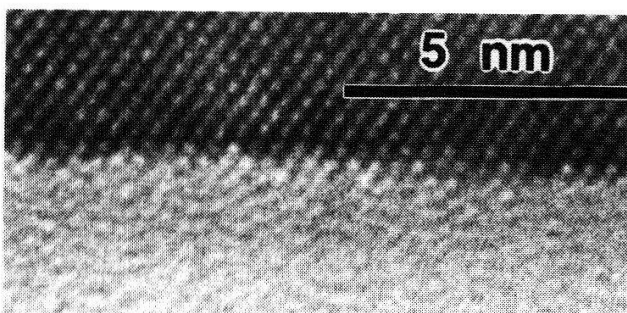


Figure 3.: Agrandissement d'une région de la figure 2.

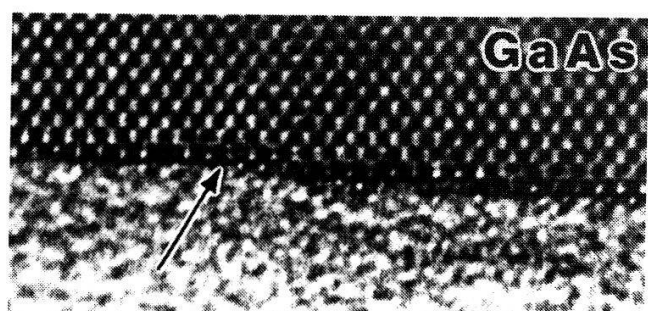


Figure 5.: Agrandissement d'une zone épaisse de la figure 4.

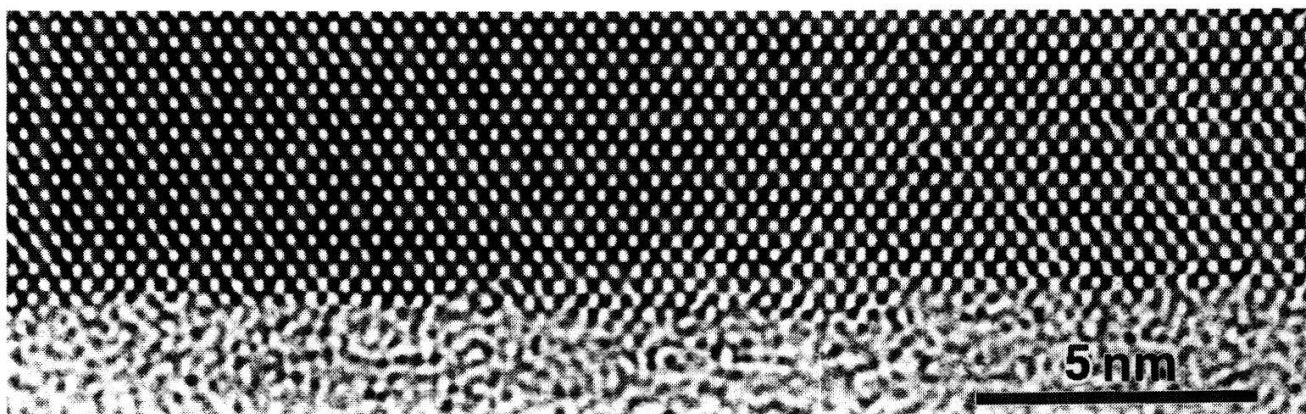


Figure 6.: Agrandissement de la zone mince de la figure 4.

3. Discussion des résultats

Les clichés de la figure 1. présentent des résultats obtenus avec des ions d'argon pour les conditions les meilleures⁽¹⁾. On peut observer sur ceux-ci que la couche de cristal modifiée par le bombardement ne dépasse pas quelques couches atomiques au maximum et en moyenne deux couches. La rugosité est par contre sensiblement plus élevée et peut atteindre jusqu'à 4 couches atomiques.

La figure 2. représente deux zones d'un même échantillon préparé avec des ions d'iode avec une énergie de 5 keV. On voit d'une part que le cristal ainsi obtenu présente une couche amorphe d'environ 1.7 nm et que le cristal en-dessous de cette couche est presque parfait. D'autre part, il n'y a pas de contraste dif-fus au niveau des couches atomiques près de la couche amorphe et la rugosité de la surface est d'environ 10 couches atomiques. La figure 3. montre un cliché haute résolution d'une zone épaisse du même échantillon et le contraste atomique est bien conservé jusqu'au bord de la partie cristalline

La figure 4. montre le résultat obtenu lorsque l'on bombarde avec des ions d'iode de 2keV. La couche amorphe a une épaisseur d'environ 1.6 nm La rugosité est plus faible (environ 5 couches) que pour des ions de 5keV d'énergie. On distingue 2 régions (agrandies dans les figures 5. et 6.) d'allures différentes: la zone épaisse (Fig. 5.) qui présente une ligne sombre au niveau des dernières couches atomiques, cela peut être dû à un effet de surépaisseur ou à une pulvérisation préférentielle en surface, et la zone mince (Fig. 6.) où le cristal est régulier jusqu'au bord avec quelques colonnes floues (coexistence amorphe/cristal).

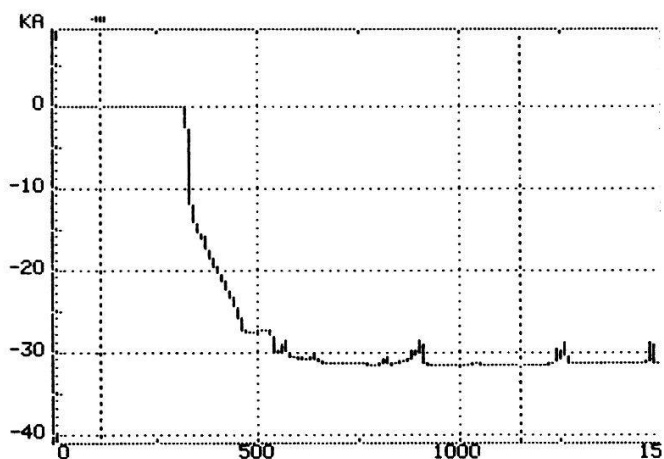


Figure 7.: Profil pour un échantillon bombardé avec des ions de 5keV d'énergie.

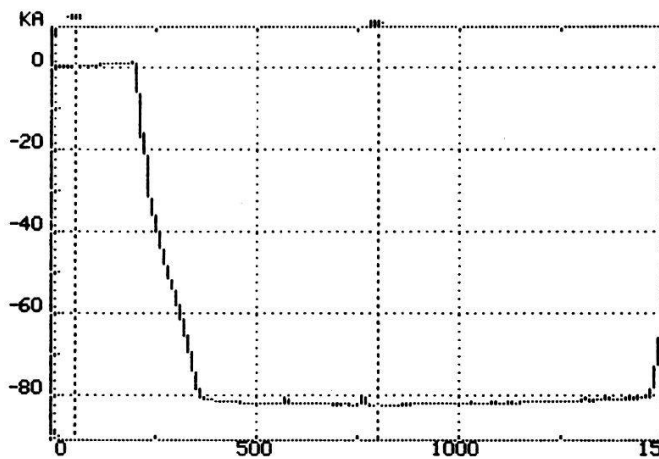


Figure 8.: Profil pour un échantillon bombardé avec des ions de 2keV d'énergie.

Les figures 7. et 8. montrent deux profils de la surface après l'attaque. Dans les conditions de travail utilisées et pour un courant de décharge identique, des ions de 5keV enlèvent environ 3 microns par heure et des ions de 2keV environ 8 microns.

4. Conclusions

Des ions de 2keV semblent donc plus efficaces que des ions de 5keV pour les conditions de travail utilisées et pour un courant de décharge identique. Ils fournissent de plus une meilleure attaque du point de vue de la rugosité. La différence entre l'iode et l'argon doit maintenant être étudiée du point de vue de leur effets respectifs à l'intérieur du cristal. Ceci ne sera possible de manière valable que lorsque l'on aura réussi à éliminer les effets de la deuxième phase de la préparation des coupes transverses. Par exemple, on peut utiliser une autre technique d'observation comme est celle des coins⁽⁴⁾ où le cristal est clivé selon deux plans perpendiculaires puis observé dans le microscope avec des électrons incidents à 45° par rapport aux faces ainsi clivées. La deuxième phase de préparation par bombardement est ainsi supprimée.

5. Références

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The Structure of the Na_2MoO_4 catalyst for water free dehydrogenation of methanol to formaldehyde

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Abstract: The Na_2MoO_4 has been found to have a peculiar catalytic behaviour. The CH_2O formation starts after a period of time stay at 670°C . Then the yield increases and reaches a maximum after some 12hrs. This work shows that the catalyst undergoes an extensive phase transformation prior to becoming active.

1. Introduction

Conventionally, formaldehyde is produced by partial oxidation or oxidative dehydrogenation of methanol. In these processes, water is formed as a by product. Sodium compounds have recently [1] been found to be active in water free formaldehyde production. Moreover, these catalysts were shown to deactivate very slowly. It was presumed that coking was the main factor of deactivation. Most of the catalytic activity could be recovered by burning the coke at high temperatures ($> 800^\circ\text{C}$). However, the change of color in Na_2MoO_4 appeared to be linked to the delayed catalytic activity; it can hardly be only explained by coking. This latter effect would hinder the catalytic activity instead of being parallel to it. In the following, we discuss the results and present the first conclusions of our current investigations on this new catalyst.

2. Experimental

The formaldehyde production is carried out at 670°C , following the heating sequence sketched in fig.1a. The activity of the catalyst during that time is shown on fig.1b. This behaviour is different from what happens when other sodium compounds (Na_2CO_3 or $\text{Na}_2\text{B}_4\text{O}_7$) are used as catalysts for the same reaction. For this investigation, samples were examined at various stages on fig. 1a (0h, 6h, 12h). The 0h sample corresponds to the time when 670°C is settled; and the 12h sample is normally the one which presents a full catalytic activity.

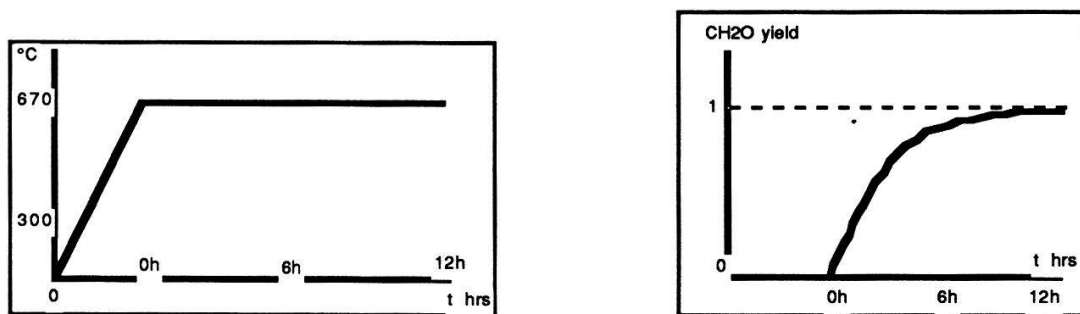


Fig. 1: a) Heating sequence. b) Catalytic activity vs time at 670°C

The formaldehyde production follows this reaction: $\text{CH}_3\text{OH} \rightarrow \text{CH}_2\text{O} + \text{H}_2$. A large amount of hydrogen is then formed. The effect of H_2 on the structure of the catalyst at reaction temperature (670°C) had to be understood. We therefore examined samples of Na_2MoO_4 which had been heated at 670°C for 12h.

3. Results

a. -Effect of heating for 6hrs at 670°C in methanol

When the catalyst bed is >10cm, the formaldehyde starts to form at this point. The powder has become a solid of black color outside and one sees an inner white part when it is broken. Our observations show that at this stage the material has undergone an extensive decomposition (fig.2). There is Na rich needlelike material stemming out from Mo rich areas. Until now, these sodium rich areas have been found to be amorphous.

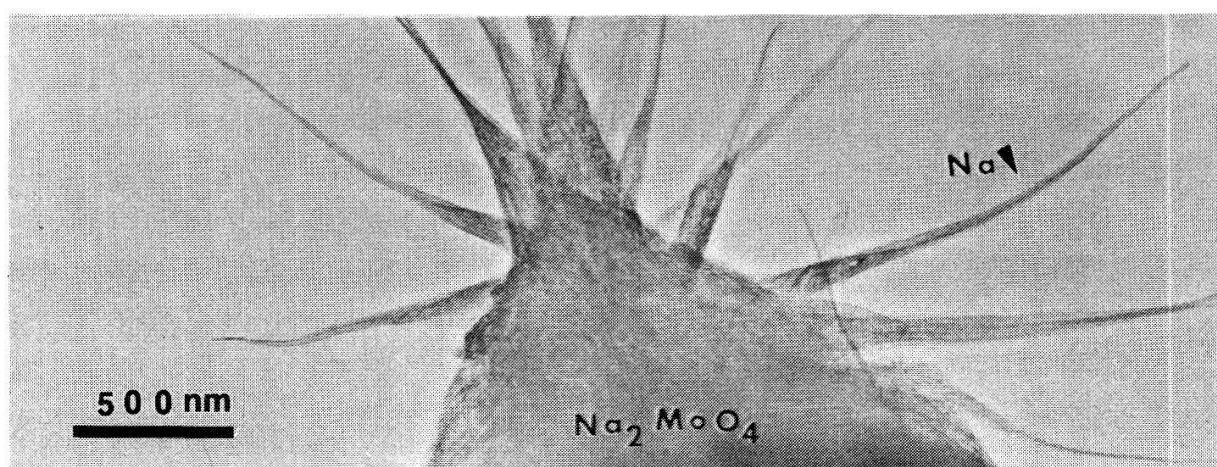


fig. 2: The catalyst after 6hrs in methanol at 670°C

c. -Heating for 12hrs in methanol

The catalyst has now become an entirely black solid, as the catalytic activity reaches its maximum. The decomposition has proceeded much further. The Na rich needles are now much bigger (fig.3) and most of the time the areas rich in Na_2MoO_4 , are covered with carbon (fig.3b). Moreover dendritic formations rich in Mo have taken place.

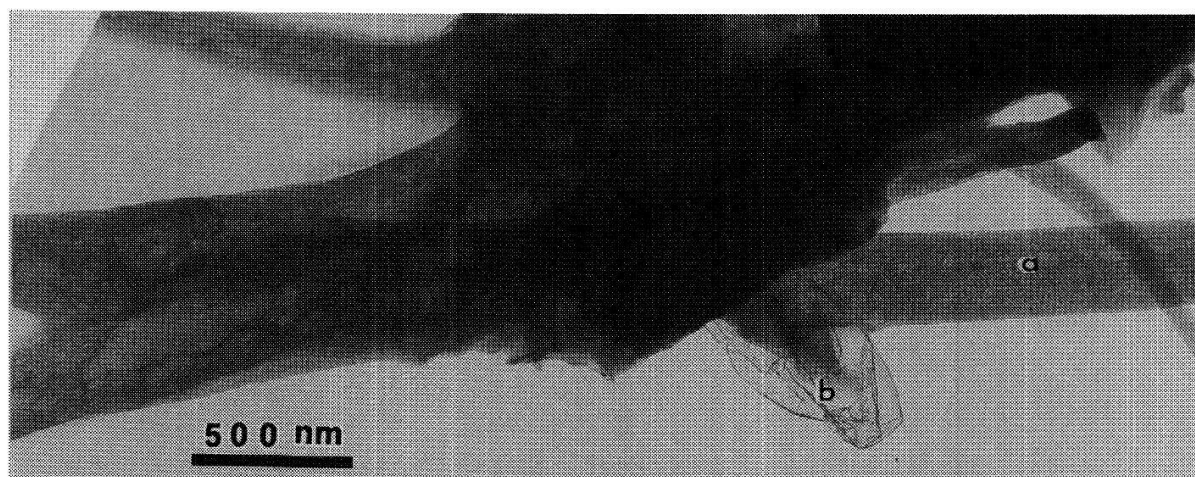


fig. 3: a)Na rich needle-like material, b) coking of the remaining Na_2MoO_4

When this material is put into water, it separates into a soluble, whitish compound and a black non soluble phase. The soluble material is mostly $\text{Na}_2\text{MoO}_4 \cdot 2\text{H}_2\text{O}$ from the initial phase. In addition we find a Na rich compound which does not contain any detectable Mo. This material appears to be microcrystalline after drying. It's structure as determined by electron diffraction seems to be that of a sodium carbonate compound. There seem to be two candidates NaCO_3 and $\text{NaCO}_3 \cdot 10\text{H}_2\text{O}$. The non soluble material is made of Mo rich phases. We have found some MoO_3 microcrystals and a material made of mixed Mo (Mo_9O_{26} , MoO_3 , ...) oxides.

d. -Heating in Hydrogen 670°C 12hrs

After these 12hrs the catalyst becomes a whitish solid in an large inner part. The black outer part is extended on less than 1mm. On fig.4, it appears that the Na_2MoO_4 has undergone transformation as well. The Na separated material bares the needlelike aspect. However the Mo rich area do not seem to separate away from the initial Na_2MoO_4 material. They are found to form an intimate mix-

ture with it (fig.4b). In the inner part of the solid, we do not notice any phase separation. All the analyzed samples exhibit the original composition.

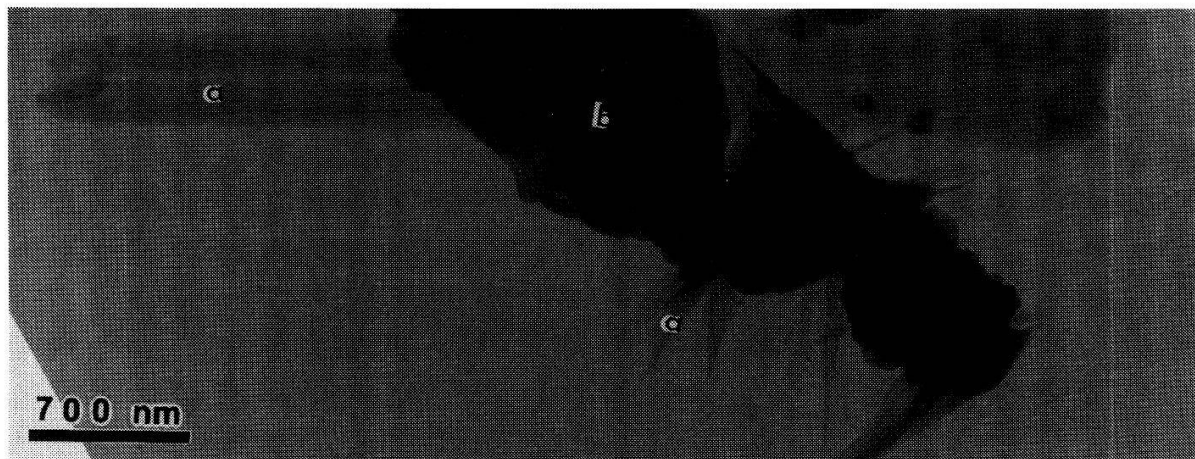


Fig. 4: 12 hours in H_2 , a) separation of Na rich areas, b) intimate mixture of Mo rich areas and original material- Na_2MoO_4

When this sample is put into water, we only find two separate phases: A non soluble compound which show small crystals of MoO_2 and microcrystals of Mo_4O_{11} of monoclinic structure. In the soluble phase we only have found the hydrated form of Na_2MoO_4 .

3. -Conclusion

These preliminary results show that the catalytic activity of Na_2MoO_4 does not start until it undergoes an extensive decomposition. From morphological point of view, it appears that Na separates in similar ways in the methanol or in hydrogen treated samples. This does not imply that we have the same phases in both cases. For the Mo rich phases there seems to be some difference: a) We do not find any dendritic formation in the H_2 treated samples. b) The Mo rich phases remain mixed with the original Na_2MoO_4 material. c) From the electron diffraction analysis, we can draw these preliminary results : -In the H_2 treated sample there seems to form MoO_2 small crystals and Mo_4O_{11} microcrystals. -In the CH_3OH treated one, lesser reduced forms of Mo oxides are produced (MoO_3 small crystals, and a mixture of MoO_3 and Mo_9O_{26} , etc... in the dendrites.

Dr. M. Prairie and M. S. Su from IGC-EPFL are gratefully acknowledged for providing the samples and for fruitful discussions.

A geometrical model of special grain boundaries in corundum.

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Abstract: A general method for determining the coincidence orientations in rhombohedral lattices is derived and applied to the interpretation of transmission electron micrographs of grain boundaries in corundum.

Metals and ceramics are used in polycrystalline form for most of their applications. Two neighbouring grains, 1 and 2, of the same phase are in coincidence orientation if the lattices of their symmetry translations have vectors in common that form a 3-dimensional lattice, called the **coincidence lattice**. The volume of a primitive cell of this lattice is an integral multiple Σ of the corresponding value for the rhombohedral lattice. The rhombohedral translation lattice 1 can always be mapped onto lattice 2 by a rotation. The **multiplicity** Σ depends on the rotation and, in general, also on the axial ratio. If c^2/a^2 is rational then one can put

$$c^2/a^2 = 3\mu/2\rho \quad , \quad (1)$$

where μ and ρ are integers such that $\mu - \rho$ is a multiple of 3 and that μ and $(\mu - \rho)/3$ have no factor in common,

$$\gcd(\mu, (\mu - \rho)/3) = 1 \quad . \quad (2)$$

Let m, u, v, w be integers such that $2u + v + w$ is a multiple of 3 and that

$$\gcd(m, u, v, (2u + v + w)/3) = 1 \quad . \quad (3)$$

Planes will be denoted by their Miller-Bravais indices, axes correspondingly by their Weber indices. The rotation with axis $[uv.w]$ and angle Θ given by

$$\tan \frac{\Theta}{2} = \sqrt{\frac{\mu w^2 + 2\rho(u^2 + uv + v^2)}{3\mu m^2}} \quad (4)$$

generates a coincidence lattice with multiplicity

$$\Sigma = f/(3f_1 f_2 f_3 f_4) \quad ,$$

where

$$f = \mu(3m^2 + w^2) + 2\rho(u^2 + uv + v^2) \quad ,$$

and

$$\begin{aligned} f_1 &= \gcd(2, m + w) \quad , \\ f_2 &= \gcd(2, m + w, u, v) \quad , \\ f_3 &= \gcd(\mu, 2f_1^{-1}u, 2f_1^{-1}v) \quad , \\ f_4 &= \gcd(\rho, 2f_2^{-1}m, m + w, 2(\mu w + \rho(v - u))(3f_3)^{-1}) \quad . \end{aligned} \quad (5)$$

It follows that Σ is independent of μ and ρ for rotations with axis parallel to the 3-fold axis of the rhombohedral lattice and for 180°-rotations with axis perpendicular to the 3-fold axis: If

$u = v = 0$ then $\Sigma = (3m^2 + w^2)/(3f_1^2)$; if $m = w = 0$ then $\Sigma = (u^2 + uv + v^2)/3$. Rotations with parameters satisfying (3) and either $u = v = 0$ or $m = w = 0$ are called **common rotations**. They have the same value of Σ for each axial ratio c/a . If c^2/a^2 is rational then there are also **specific rotations**. Their parameters satisfy (3); their multiplicities depend on c/a .

The following lower bound for the multiplicity of specific rotations as a function of μ and ρ can be derived from (5):

$$\Sigma \geq \sqrt{8\mu\rho}/3 \text{ if } \mu \text{ and } \rho \text{ are odd, } \Sigma \geq \sqrt{2\mu\rho}/3 \text{ otherwise.} \quad (6)$$

This bound can be used to compute tables of all specific coincidence rotations with c/a in a given interval and multiplicity up to a given value Σ_c .

A given relative orientation of 2 grains can be described by different rotations due to the trigonal symmetry of the rhombohedral lattice. These rotations form an equivalence class. Exactly one rotation in each class, called the representative $\{muv.w\}$, satisfies the conditions:

$$u \geq 0, \quad v \geq 0, \quad w \geq 0, \quad (7)$$

$$m \geq w, \quad m \geq \sqrt{\rho/2\mu}(u + v), \quad (8)$$

$$\begin{aligned} v &\geq u & \text{if } w &= 0, \\ v &> u & \text{if } w > 0 & \text{ and } m = \sqrt{\rho/2\mu}(u + v). \end{aligned} \quad (9)$$

Eq. (7) defines a spherical triangle bounded by 2 mirror planes of lattice 1 and the plane perpendicular to its 3-fold symmetry axis. This triangle comprises 1/12 of the full solid angle and is called the standard spherical triangle or SST. Each rotation angle occurring in an equivalence class occurs also with an axis in the SST. The representative has its axis $[uv.w]$ in the SST and (because of (8)) the smallest angle occurring in the class. If there are several such rotations then (9) makes a unique choice.

Many classes contain 180°-rotations. Examples are given in Tables 1 and 2, which give the following information: 1) short symbol containing Σ , 2) representative, 3) Miller-Bravais indices of the planes perpendicular to the axes of 180°-rotations in the SST.

Σ	Representative			Miller-Bravais indices		
	Θ^0	m	w	of symmetry planes		
3	60.00	3	3	1 0 . 0	0 1 . 0	0 0 . 1
7	38.21	5	3	4 1 . 0	1 4 . 0	
13	27.80	7	3	5 2 . 0	2 5 . 0	
19	46.83	4	3	7 1 . 0	1 7 . 0	
21	21.79	9	3	2 1 . 0	1 2 . 0	

Table 1: The equivalence classes of common rotations with $\Sigma \leq 30$. The representatives have the form $\{m 0 0 . w\}$.

μ	ρ	c/a	Σ_s	Σ	Representative			Miller-Bravais indices of symmetry planes	
					Θ°	m	u	v	w
34	7	2.699	8	8	86.42	1	0	2	1
49	10	2.711	11	14	75.52	5	0	7	5
64	13	2.717	14	14	94.10	13	0	32	13
15	3	2.739	7	7_1	85.90	1	0	2	1
				7_2	85.90	3	6	0	3
				$11a_1$	68.68	1	1	0	1
				$11a_2$	68.68	3	0	3	3
				$11b$	95.22	1	0	3	0
				$13a$	57.42	2	0	3	0
				$13b_1$	94.41	6	0	15	6
				$13b_2$	94.41	2	5	0	2
56	11	2.763	12	12	94.78	11	0	28	11
				13	85.59	1	0	2	1

Table 2: The equivalence classes of specific rotations with $\Sigma \leq 14$ and $7.25 \leq c^2/a^2 \leq 7.65$. Σ_s is the value of the lower bound (11) rounded to the next higher integer.

Corundum ($\alpha\text{-Al}_2\text{O}_3$), the most important oxide ceramic material, has space group $R\bar{3}c$. Its rhombohedral lattice has the axial ratio $c/a = 2.730$. Haematite (Fe_2O_3) with $c/a = 2.732$ is of the same structure type. In both cases, the most common types of twins are the **basal twin** with twinning plane (00.1) and the **rhombohedral twin** with a {01.2} plane [1,2]. The description of these twins by the coincidence rotations $\Sigma 3$ in Table 1 and $\Sigma 7_1$ in Table 2 makes it possible to predict the possible Burgers vectors of dislocations in the twinning plane. They are vectors of short length of the DSC lattice, which can be obtained from the coincidence lattice by a reciprocity relation [3]. Burgers vectors of dislocations in twin boundaries have been determined for basal twins in [4], for basal and rhombohedral twins in [5]. They have the predicted form. A multiplicity $\Sigma = 8$ instead of $\Sigma 7_1$ was proposed in [2] for the rhombohedral twin because systematic tables of all possible coincidence orientations were not available [5]. For the same reason, TEM observations on $\alpha\text{-Al}_2\text{O}_3$ were interpreted in [6] using tables for hexagonal lattices. These observations have been revisited in [7] on the basis of the present results.

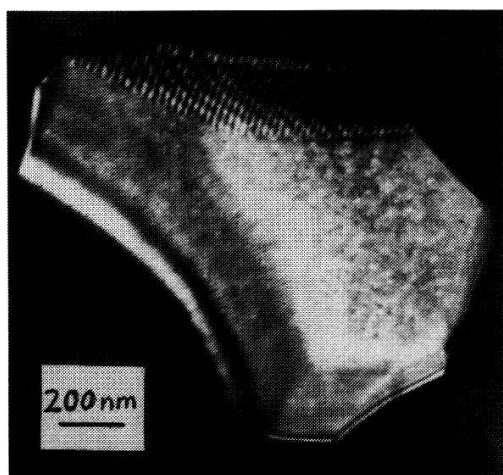
Networks of dislocations are expected in a grain boundary if the rotation connecting the two adjacent grains is a specific rotation because of the mismatch due to the difference between the experimental value of c/a and the value given in Table 2. Additional dislocations are expected if the rotation slightly deviates from a specific or common rotation. This explains why Shiue and Phillips [5] always found dislocations in the boundary of rhombohedral twins but only sometimes for basal twins.

Brandon [8] estimated that the structure of a coincidence boundary will locally be preserved in cubic materials as long as the angle Θ of the deviation from a coincidence orientation satisfies

$$\Theta \leq 15^\circ / \sqrt{\Sigma} . \quad (10)$$

It was suggested in [7] to use this criterion also to discuss the distribution of relative orientations in corundum. If the grains are oriented at random then one expects 0.57% low angle boundaries, i.e. boundaries satisfying (10) with $\Sigma = 1$ [9], 0.23% of boundaries satisfying (10) for a common rotation with $1 < \Sigma \leq 36$, and 1.19% of boundaries satisfying (10) for a specific rotation with $c/a = 2.739$ and $1 < \Sigma \leq 36$. (The restriction $\Sigma \leq 36$ was chosen because the Burgers vectors can become too small for the distribution to be visible in TEM if Σ becomes larger.)

S. Lartigue found [10] that the frequency of such special boundaries was compatible with the expected value for pure $\alpha\text{-Al}_2\text{O}_3$ and for low angle and common boundaries in $\alpha\text{-Al}_2\text{O}_3$ doped with 500 ppm of MgO. She analysed 56 boundaries in the doped $\alpha\text{-Al}_2\text{O}_3$, 23 in as pressed samples and 33 in deformed samples [7]; 3+5=8 among them were high angle boundaries of the specific type defined above, i.e. 14 times more than expected for a random distribution. She observed a network of dislocations in 6 among these 8 boundaries. It is concluded that certain high angle coincidence boundaries are highly favored in $\alpha\text{-Al}_2\text{O}_3$ doped with small amounts of MgO.



Dark field transmission electron micrograph of a small grain in the as pressed sample of doped $\alpha\text{-Al}_2\text{O}_3$ showing periodic networks of dislocations (Courtesy S. Lartigue).

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SILICIDE FORMATION FOR Cu ON a-Si:H

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Abstract : we have measured by Rutherford Backscattering Spectrometry (RBS) the rate of formation of Cu_4Si in a-Si:H at four temperatures between 160 °C and 200 °C. The results show that the Cu_4Si thickness is proportional to $t^{1/2}$ indicating that the process is controlled by diffusion.

1. Introduction

The silicide formation in monocrystalline Si (c-Si) has been extensively studied and is well documented [1]. It is not the case for micro- and nanocrystalline Si ($\mu\text{c-Si}$ and nc-Si resp.) and amorphous Silicon (a-Si), although these materials are of great technological importance [2]. The diffusion of metallic ions implanted in a-Si has been investigated [3,4] and the formation of Pd_2Si in a-Si:H has been reported without indication of its kinetics [5]. Nemanich et al. [5] and Vanecek [6] have suggested that hydrogen in a-Si:H might be important in the silicide formation and/or diffusion processes. To our knowledge, the present work is the first systematic study of the kinetics of silicide and of the diffusion processes in nc-Si:H and a-Si:H. a-Si:H is unstable above 600 °C [7] but this difficulty could be overcome by choosing Cu which is a fast diffuser in Si [4,5]. Cu-silicide formation and diffusion processes are expected to occur much below the 600 °C limit [4,5]. We report here the results of our investigations in Cu_4Si formation in a-Si:H substrates of - as produced - hydrogen concentration. We have used the Rutherford Back Scattering (RBS) technique [8] which is well adapted to this type of study.

2. Experimental

The a-Si:H/c-Si substrates were prepared by the Silane based VHF-Glow Discharged (VHF-GD) method which is a novel high rate deposition method recently developed at IMT [9]. This method increases the deposition rate without any degradation of the material quality. The deposition parameters are listed in ref. [10].

The substrates were first annealed at 200 °C in UHV ($p < 1.E-8$ torr) for 30 min. and then cooled down for one hour, a treatment which is not expected to modify the H-concentration. Without breaking the UHV a 4000 to 5000 Å thick Cu-layer was then deposited by evaporation on top of the Si substrate. No subsequent Si-diffusion through Cu grain joints has been observed (Type C diffusion [11]). Then the samples were transferred into the RBS chamber ($p < 5.E-7$ torr) where they were fixed on a Ag backing that could be heated by IR radiation. The temperature variations could be performed within less than 50 s. and the temperature could be kept constant within ± 2 °C during the annealing. After each heat treatment, the samples were exposed to the MeV alpha-beam, 0.5 mm in dia., produced by our Van de Graaff accelerator. Backwards (150 °) elastically scattered alphas were detected by a surface barrier Si detector (RBS spectra). The data were analysed with our own "RBSERA" computer code.

3. Results

The RBS spectra of Fig. 1 show clearly the formation of Cu_4Si : spectrum 1 comes from the unannealed Cu/a-Si:H sample, spectra 1 and 2 from the annealed sample at 185 °C for 11 and 30 min. resp. The step on the right part of these last two spectra is due to the silicide. In fig. 2 the thickness x of Cu_4Si plotted versus the square root of the annealing time t at different temperatures, shows a linear behaviour : $x = (k(T) \cdot t)^{1/2}$ where $k(T)$ is the rate of formation. This result indicates that this process is controlled by diffusion [1]. The temperature thres-

hold for Cu_4Si formation is found to be around 150°C . From the Arrhenius plot of $k(T) = k_0 \cdot \exp(-E_a/kT)$ (k = Boltzmann constant) shown in fig. 3, we obtain a value of 1.9 eV for the activation energy E_a . One can expect E_a to be dependent on the H concentration and the structure of the Si layer (a-Si:H, nc-Si:H). The investigation of these problems and of the H affinity of the diffusing metal is in progress.

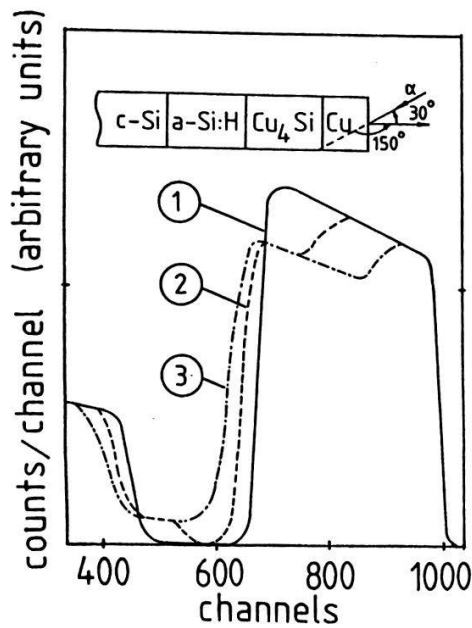


Fig. 1 : see text

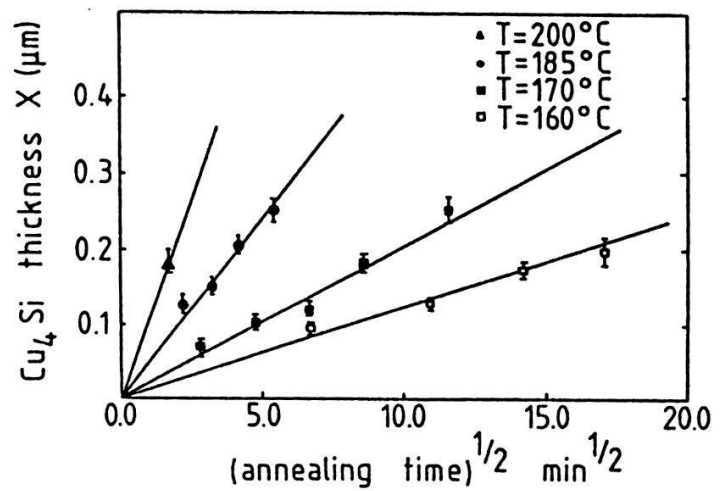


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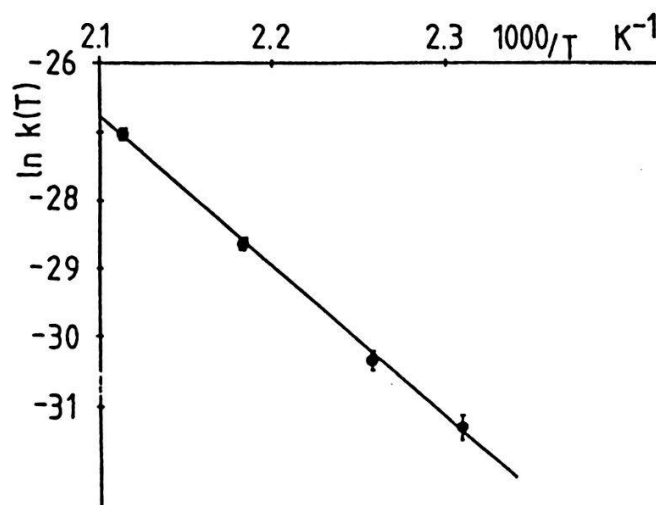


Fig. 3 : see text

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Macroscopic Quantum Tunneling and Thermal Activation in Small-Area Josephson Tunnel Junctions and a dc-SQUID

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Abstract : We report measurements of thermal activation (TA) and macroscopic quantum tunneling (MQT) out of the zero-voltage state in a dc-SQUID. We observe that the crossover from MQT to TA regions strongly depends on the magnetic flux bias, and that the TA rates are smaller than those predicted by classical theories. We also report preliminary MQT studies in a small-area SIS (superconductor-insulator-superconductor) Josephson tunnel junction capacitively coupled to an SIN (superconductor-insulator-normal metal) tunnel junction.

Introduction

In a current-biased Josephson junction, the relevant macroscopic variable is the phase difference δ between the two superconductors. The junction is described as an ideal non-linear inductor that follows the Josephson phase relations, shunted by a resistance R and a capacitor C (RSJ model). In this model, the evolution of δ is similar to the motion of a particle with mass $C(\phi_0/2\pi)^2$ in a one dimensional washboard potential: $U(\delta) = (-I_0\phi_0/2\pi)[\cos\delta + (I/I_0)\delta]$, with a friction coefficient $R^{-1}(\phi_0/2\pi)^2$ [1]. I is the applied current, I_0 is the critical current and ϕ_0 is the flux quantum. In the zero-voltage state the phase is trapped in a metastable potential well of height: $\Delta U = (2\sqrt{2}I_0\phi_0/3\pi)(1 - I/I_0)^{3/2}$. The frequency of small oscillations at the bottom of the well is $\omega_p = (2\pi I_0/C\phi_0)^{1/2}[1 - (I/I_0)^2]^{1/4}$, and the damping is characterized by $Q = \omega_p RC$ ($Q \gg 1$ implies low damping). When the device is current-biased close to the critical current, escape from the well can occur by TA over the barrier with a rate given by [2]:

$$\Gamma_t = a_t(\omega_p/2\pi)\exp(-\Delta U/k_B T) \quad (1)$$

where the prefactor a_t is dependent on the damping. At low temperatures δ tunnels through the barrier (MQT). For low temperatures the escape rate is [1] :

$$\Gamma_q = a_q(\omega_p/2\pi)\exp[-7.2\Delta U/\hbar\omega_p(1 + 0.87/Q + \dots)] \quad (2)$$

where $a_q = [120\pi(7.2\Delta U/h\omega_p)]^{1/2}$.

A dc-SQUID is a superconducting ring interrupted by two Josephson junctions. Here the relevant variables are the two phases δ_1 and δ_2 , (phase difference at each junction). The dynamics of a dc-SQUID is similar to that of a particle moving in a two-dimensional washboard potential [4] with numerous wells and saddles in the δ_1, δ_2 plane. The potential surface is tilted according to the current bias, while the flux bias shifts the locations of the wells and saddles. The thermal activation rate is obtained from the one dimensional case [2] with the corrections to the prefactor a_t in Eq. 1 given by Brinkman [3]. The MQT rates, for a low inductance dc-SQUID can be obtained from the work of Chen [5], where it is shown that the single junction escape rate given by Eq. 2 is a good approximation.

The dc-SQUID measurements

The dc-SQUID studied had window junctions made of $PbInAu - In_2O_3 - PbAu$ with typical dimensions of $0.8\mu m^2$ and SQUID loop area of $0.2\mu m^2$. A capacitance per junction of $(80 \pm 20)fF$ was calculated from the geometry and oxide properties of the insulating barriers and was in accordance with SQUID resonance measurements. The loop inductance as determined from the SQUID critical current modulation depth, was found to be $L = (2.4 \pm 0.1)pH$. The critical current at zero magnetic flux bias ($f=0$) was: $I_c = 2I_0 = 107.2\mu A$ and for an applied flux of $1/2\phi_0$ ($f=1/2$): $I_c = 9.6\mu A$.

Distribution of switching currents $P(I)$ are obtained by repeatedly ramping the SQUID bias current and recording the values at which a non-zero voltage appears. Typically a distribution consists of 50,000 events. From $P(I)$ one extracts the escape rate. Details of the measurement and the sample fabrication can be obtained elsewhere [6]. Noise isolation was a major concern in this experiment. The data was taken at very low frequency to allow thermal equilibrium at all the data points. Data was taken in the range of 50mK to 1.3K at several values of flux bias to check for flux noise. Fig. 1 shows the peaks of the $P(I)$ distributions ($\langle I \rangle$) for $f=0$, and $f=1/2$, as a function of the temperature (T). At high temperatures $\langle I \rangle$ is linear with T , while at low temperatures the data is T independent. One finds that, T_c , the crossover temperature from MQT to TA regions, is substantially smaller for $f=1/2$ than for $f=0$ indicating that the tunneling rate changes strongly with the flux bias. Our computer simulations using classical models [3] of the thermal activation rates (curve TA in Fig. 1) show that our rates are much smaller than the theoretical predictions. It is as if the potential barrier were enhanced by a factor of 2.5 (curve MTA). Quantum corrections to the thermal rate (curve MTA^*) produce only a small change in the above picture. The low temperature MQT regime can be fitted with the usual expressions for the rate, showing that the anomaly is present only in the TA region. An extensive

discussion can be found elsewhere [6].

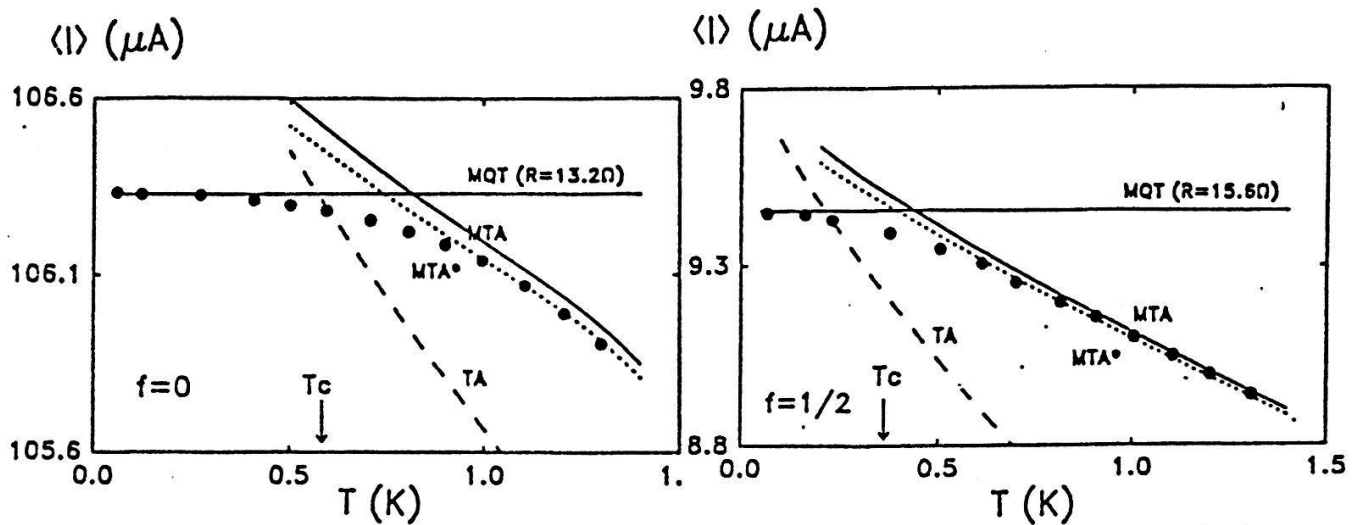


Fig. 1 Peak of $P(I)$ vs Temperature for $f=0$ and $f=1/2$. MQT dominates below T_c . The classical predictions for the thermal activation (TA curve) are much smaller than the observed rates. It is as if the potential barrier were enhanced (MTA curve).

The SIS Josephson Junction coupled to an SIN junction

Using standard microfabrication techniques, we have made a system consisting of an SIS Josephson junction capacitively coupled to an SIN junction. The junction structure was similar to those of the dc-SQUID described above. The junction size was $1.0\mu m^2$, the counter electrode for the s-i-n was made of Cu, and the two junctions were coupled by parallel Cu plates $(300 \times 400)\mu m^2$. Our computer simulations of the mentioned system shows that at high frequencies it behaves similarly to a single junction with a variable shunt resistance or variable damping. This resistance can be adjusted at will by changing the dc-bias of the SIN junction. The simulated SIS I-V characteristics show very little change with the SIN bias.

The measured I-V characteristics of the SIS junction was that of a very high quality device, and as predicted it showed no noticeable change with the SIN bias. The SIS device had a critical current $8.0\mu A$ and a normal state resistance of 100Ω . The SIN junction resistance was 1040Ω for zero bias, and 25Ω for a bias above the gap, which yields a damping parameter Q range from 16 (low damping) to 0.4 (high damping). The measurements of the escape rate were similar to those in the dc-SQUID experiment. Fig. 2 shows the measurements for zero SIN bias (circles) and some MQT and TA computer simulations for different values of the shunt resistance. At low temperatures we observe the temperature independent regime MQT and the crossover to the high temperature TA region. We see that the data agrees very well with the theoretical predictions for the TA

and MQT escape $P(I)$ distributions. Fig. 3 shows the shift of the peak position of $P(I)$ with the SIN bias. The data has a peculiar structure, especially pronounced at the SIN gap bias. At the moment we are modeling possible mechanisms that could produce the observed shift of $P(I)$ with the SIN bias.

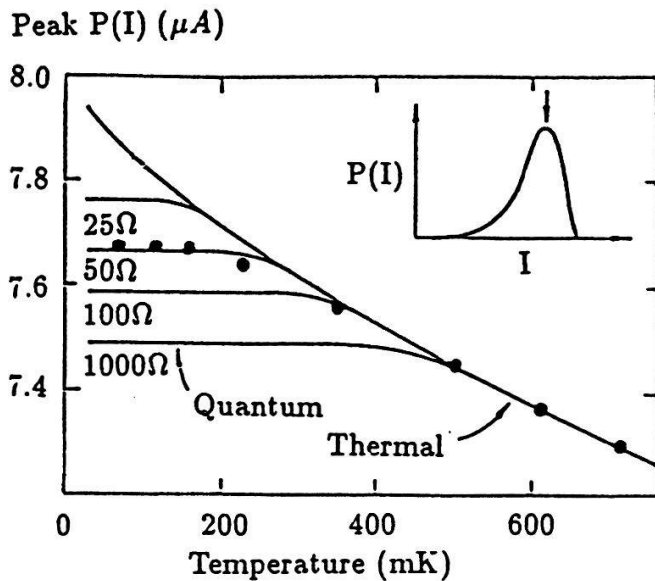


Fig. 2 $\langle I \rangle$ vs Temperature at zero SIN bias. Solid lines are simulations.

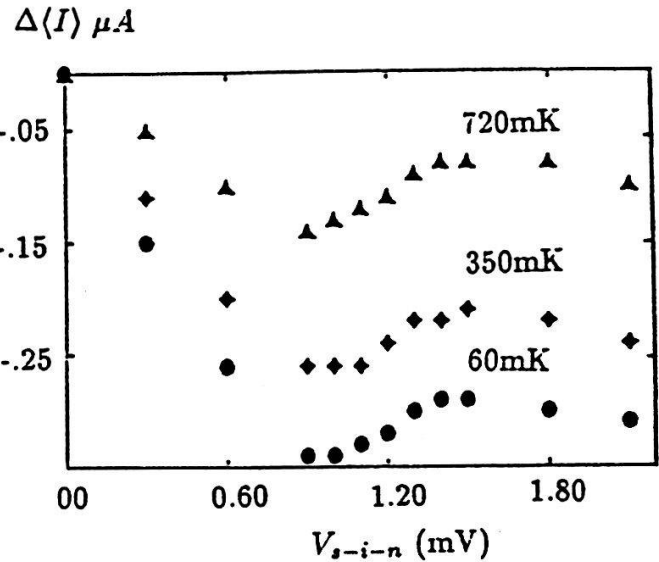


Fig. 3 Shift of $\langle I \rangle$ vs SIN bias at three temperatures.

Conclusions

We have performed MQT and TA measurements in two novel systems, where we can vary a parameter in-situ. We have observed the crossover from the MQT to TA regions. In the case of the dc-SQUID the critical temperature is a strong function of the flux bias, and the TA rates are smaller than those predicted by classical theories.

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Phase-Transition and Local Mobility of a Polymer Chain

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We have investigated the temperature-dependence of the local mobility of the poly-N-isopropylacrylamide chain (poly-NIPAM) by measuring the time resolved fluorescence-depolarization of fluorescein-isothiocyanate (FITC) attached covalently to the polymer chain (molecular weight: 300,000, degree of labelling: 5 labels per chain). Poly-NIPAM undergoes a phase-transition in water: it is soluble at temperatures below 31°C, but precipitates upon subsequent heating.

The information on the changes of the local mobility of the chain accompanying the phase transition is contained in the anisotropy $r(t)$ of the polarization of the label fluorescence [1]. In the simplest case, $r(t)$ is a single exponential $r(t) = r_0 \cdot \exp(-t/\tau_r)$, where $\tau_r = 1/6D_r$ (D_r is the rotational diffusivity). In present experiments, $r(t)$ exhibits a non-exponential behavior. Satisfactory fits have been obtained with a sum of two exponentials. The relaxation time of the fast component of $r(t)$ is $0.5\text{ns} \pm 0.2\text{ns}$ in the whole temperature range. So it seems unlikely that it represents the motions of the chain. It possibly originates from restricted reorientational motions of the dye molecule. The relaxation time of the slow component rises from 5ns below 31°C to 13ns above the phase transition temperature, which we interpret as a reduction of label mobility. Figure 1 shows the temperature dependence of the reduced rotational diffusivity $D^* = D_r \cdot 6\eta/kT$ [3]. The measured D^* is to be compared with the value of a free label ($\approx 1\text{nm}^3$), and the reduced diffusivity a rigid polymer coil of the given molecular weight would have ($\approx 7 \cdot 10^{-5}\text{nm}^3$).

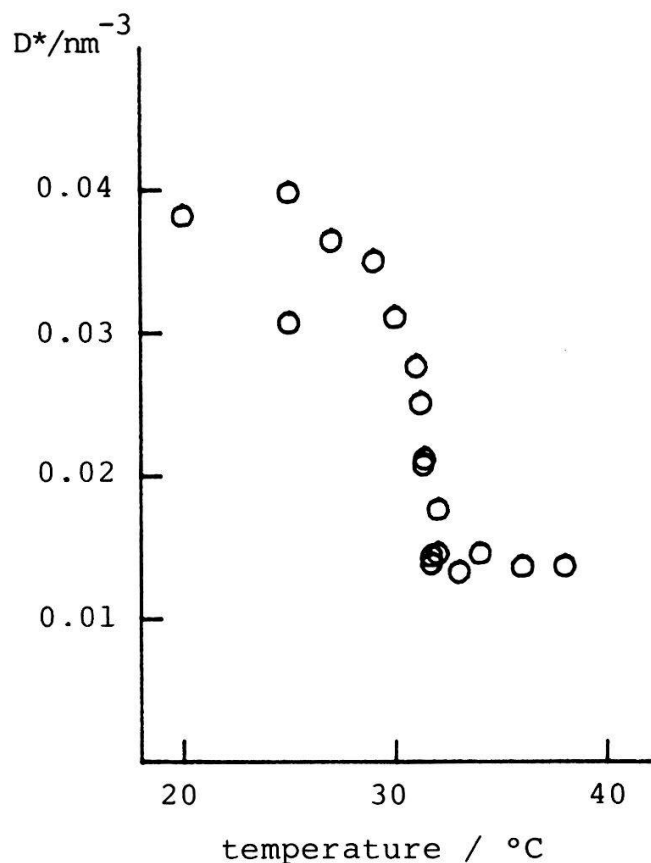


Figure 1.

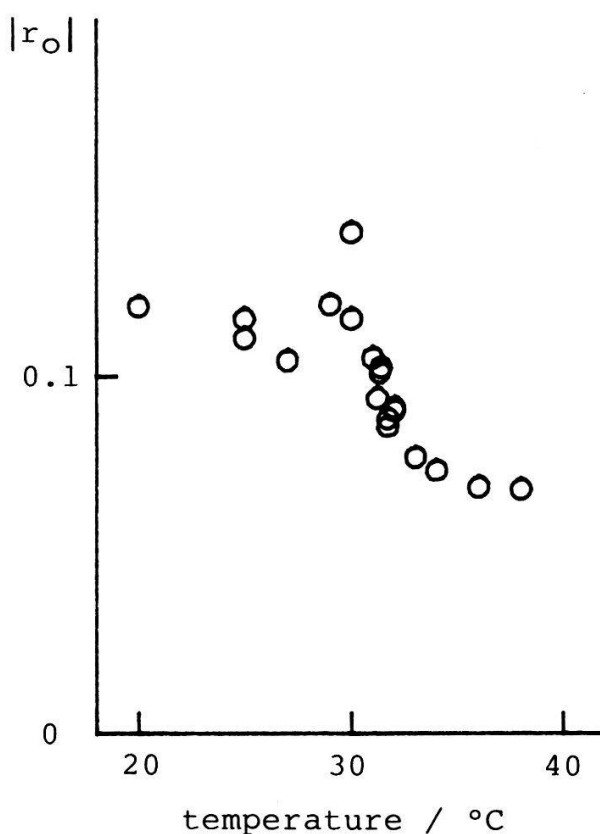


Figure 2.

In Figure 2 the initial value $r(0)$ of the anisotropy is shown to decrease by 30% at 31°C. This behavior can be attributed to an increase of the non-radiative energy transfer [2] between labels contained in one polymer macromolecule.

Both findings, i.e. the reduction of the label mobility and the enhancement of non-radiative transfer suggest the following picture of the microscopical consequences of the phase transition: Below 31°C a polymer molecule is in the state of flexible expanded coil, upon increase of temperature it collapses into a dense globule.

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- [3] So defined D^* is the inverse volume of a freely rotating rigid equivalent sphere with the rotational diffusivity D_r .

XPS STUDY OF AMINO ACID ADSORPTION TO TITANIUM SURFACES

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ABSTRACT: Titanium is used for implants in surgery. The metal spontaneously forms an oxide at the surface. Proteinacious tissue is observed to adhere strongly to the Ti surface. The purpose of this study is to understand the conditions under which amino acids bind to the Ti (oxide) surface and the mechanism(s) by which bonding occurs. Amphoteric behavior of amino acids and the oxide results in complex formation based on the relative pK values of the binding species. Adsorption of cysteine in salt solution vs. pH was monitored by X-ray photoelectron spectroscopy (XPS). Adsorption maxima and minima coincide with regions of assumed complex formation.

INTRODUCTION

The titanium surface spontaneously forms an oxide upon which adsorbed water dissociates forming two distinct hydroxyl groups of acidic and basic character. Basic OH groups can adsorb H^+ according to the reaction $TiOH + H^+ \rightleftharpoons TiOH_2^+$, while acidic surface hydroxyls become deprotonated by the reaction $TiOH \rightleftharpoons TiO^- + H^+$. Two acidity constants define the chemical equilibrium of the surface:

$$pK_{a1} = -\log \left[\frac{[H^+][TiOH]}{[TiOH_2^+]} \right] \quad pK_{a2} = -\log \left[\frac{[H^+][TiO^-]}{[TiOH]} \right]$$

where the pKa of an acid is the pH at which it is half dissociated (Henderson-Hasselbalch equation). The net charge on the titanium surface is zero at a specific pH (z.p.c.) which is the average of pKa₁ and pKa₂. The above chemical equilibrium can be visualized as shown in Figure 1 (the computer program "MICROQL"^[1] by Westall is used). PKa values of 3.77 and 6.62 (rutile surface, 1 M NaClO₄)^[2] and a z.p.c. of 5.2 were used to calculate the concentration of the three species $TiOH_2^+$, TiO^- and $TiOH$ as a function of pH.

Amino acids are also amphoteric and thus can act both as proton donors and acceptors. The amino ($-NH_2$) group is basic while the carboxyl group ($-COOH$) is acidic. Amino acids exist in solution in the form of dipolar ions, i.e zwitterions. The amino acid cysteine has an uncharged, polar R group containing a thiol ($HS-$) group which also readily donates protons. Thus the pKa's of these three functional groups determine the ionization state of cysteine, these being

$pK_{\text{COOH}} = 1.71$, $pK_{\text{HS}} = 8.33$ and $pK_{\text{NH}_2} = 10.78$ [3]. The resulting isoelectric point of cysteine falls at approx. pH 5.0. The cysteine speciation diagram (Fig 2) is obtained in the same way as for the Ti surface (computer program "MICROQL"^[1]) and shows the concentration of ionized species in a 0.37 M solution of cysteine as a function of pH.

METHODS

Cysteine was adsorbed for 6-12 hours from a 0.37M solution in 1M NaCl (pH 0.5-12.8) onto Ti plates which were chemically etched, mechanically polished (SiC, 1200 grit), rinsed and ultrasonically cleaned in bi-distilled H₂O. Post-adsorption rinsing and ultrasonic cleaning in salt solution and bi-distilled water insured detection of strongly bound cysteine. Adsorption was determined by XPS by monitoring the cysteine sulfur signal and the titanium oxide peak. Theoretical calculation of overlayer thickness was performed based on estimated sulphur atom density of the overlayer, relative electron mean free paths and signal intensity (peak area after linear background subtraction).

RESULTS

XPS spectra showed the chemical shift of Ti to Ti oxide (Ti(IV)), while no shift occurred to indicate an ionic state for S. Sulphur in the cysteine powder and adsorbed cysteine was detected at binding energies between 163.8-164.2 eV. This suggests the possible presence of di-sulfide bonds (163.8 eV) and hence oxidation of cysteine to cystine, but the exact location of the S2p peak was often obscured due to low sulfur concentrations and noise. The spectra also contained the normal hydroxyl and oxide oxygen peaks, as well as the C, O and N signals from the amino acid^[4]. Gross estimations in the overlayer thickness calculation enabled the determination of adsorbed cysteine thickness, as shown in Fig 3, where the unit in the figure is 1nm. Two distinct cysteine adsorption peaks occur, one in acidic (maxima pH 3-4) and one in basic (maxima approx. pH 10) environments. An adsorption minimum occurs around neutral pH, with no adsorption at extreme low and high pH's.

DISCUSSION

Extreme low and high pH produces like charges on the Ti surface and cysteine molecules, preventing adsorption. Adsorption in acidic pH most likely occurs between the neutral H₂L^{+/-} and basic TiOH species, probably through the deprotonated carboxyl (COO⁻) group. Complex formation probably occurs via a ligand replacement mechanism, as suggested by Wirz^[1], Schindler^[5], Kennedy^[6] and Boehm^[7], where basic TiOH dissociates as OH⁻ (rather than adsorption of H⁺) and can be exchanged for other anions. These works refer to Ti oxide powders of rutile and anatase. The basic adsorption maximum coincides with the occurrence of the negatively charged HL⁻ cysteine species and the acidic TiOH species. Deprotonation of the thiol group apparently drives the adsorption between the two negatively charged species via either (1) co-adsorption of small solution cations and involving electrostatic interactions, as observed by

Van Dulm et. al.^[8] on polystyrene surfaces; or (2) the amino (NH_3^+) group and TiO^- surface species by chemisorption^[7] or surface complexation^{[5][6]}, where amino acid (cat)ions replace the surface H^+ .

CONCLUSION

Adsorption and bonding of amino acid to the Ti hydroxide surface is a strong function of pH. Two distinct adsorption mechanisms exist for cysteine. Bonding can be explained by complex formation between the amphoteric species.

The authors would like thank Prof. Schindler, Universität Bern, for the chemical equilibrium computer program, MICROQL.

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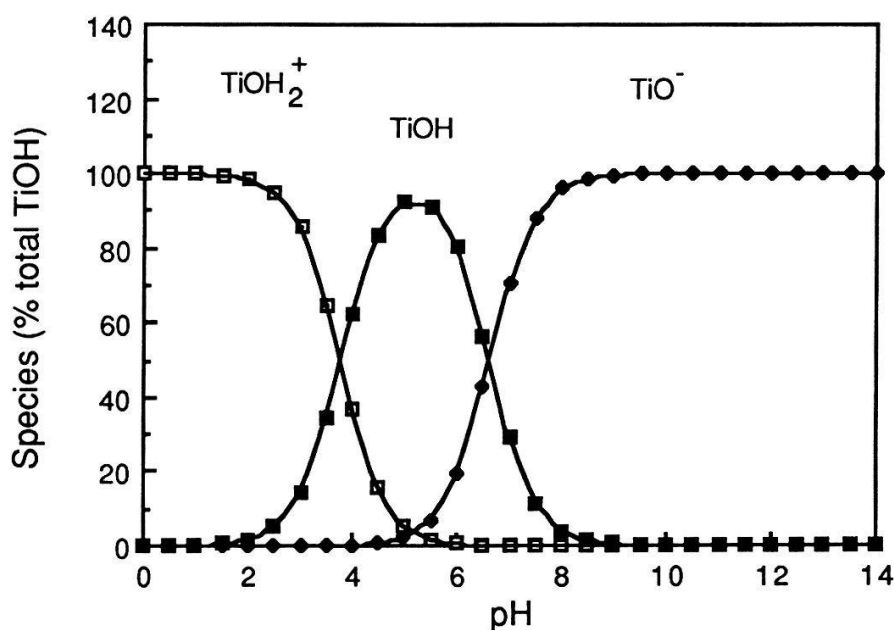


Fig 1 TiOH speciation diagram indicating pH regions of charged and neutral species.

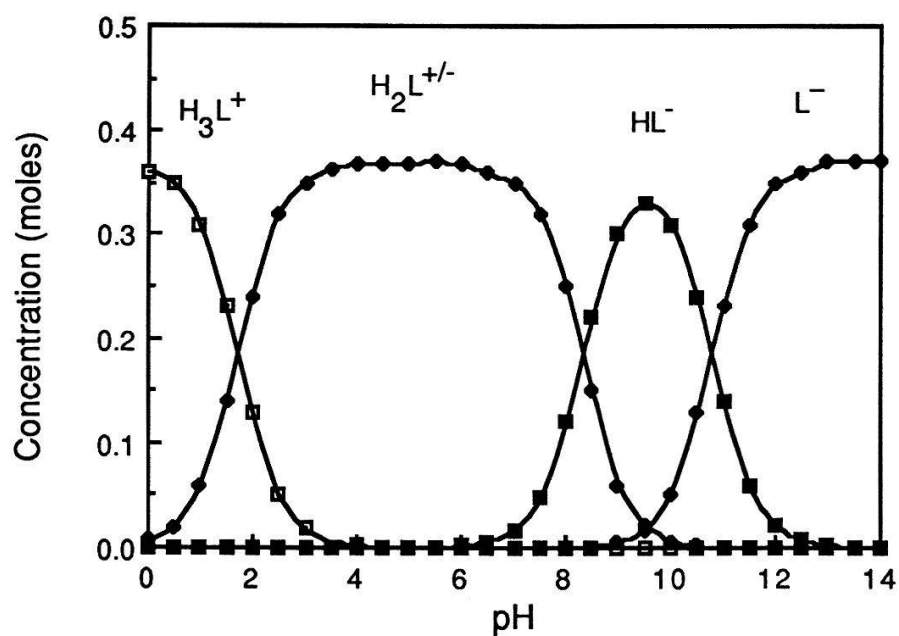


Fig. 2 Cysteine speciation diagram indicating concentration of charged species in a 0.37M solution.

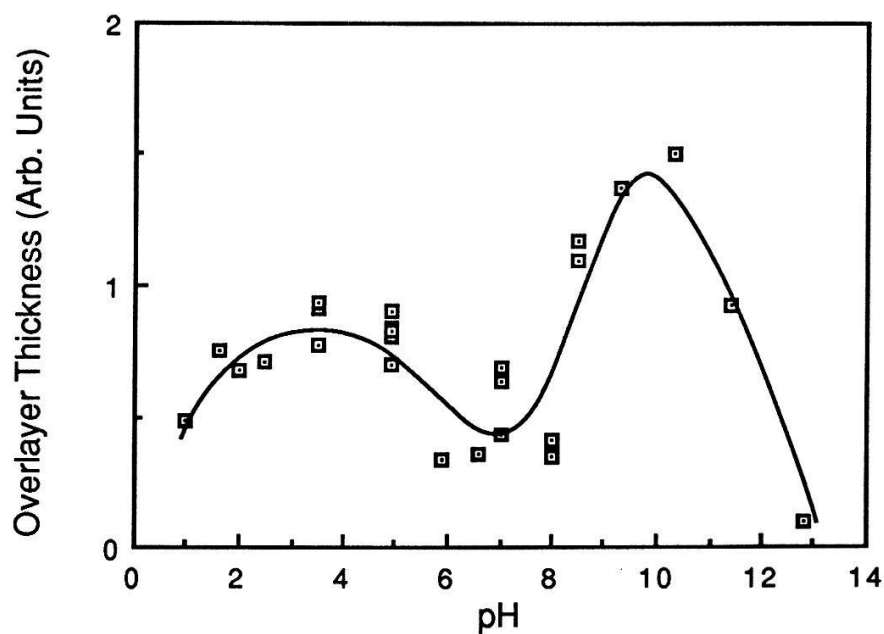
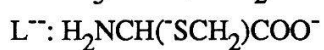
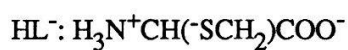
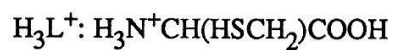


Fig 3 Cysteine adsorption vs. pH as determined by XPS analysis.

Extremal properties of dendritic patterns : biological applications

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Abstract

Recent experiments indicate that stable agglomerates of metallic balls in an electric field can have a fractal geometry and a dendritic structure. Further it has been shown, that these patterns satisfy a variational principle. We compare the geometry of these optimal patterns with dendritic structures of biological systems, e.g. the nervous system, roots. We discuss the relationship between the variational principle and the function of these roots.

1 Introduction

Dendrites are ramified, simply connected patterns. They often are self-similar in a certain range of scales/1/. Particularly for living beings they seem to be of importance. The dendritic geometry is the basic geometry of roots, ramified nerves, arteries, lymphvessels, etc.. There is also a large class of open physical systems, which provide dendritic structures, e.g. breaklines of hard materials, river systems, electric lightnings. Over the past several years, the Hele-Shaw system/2/, dielectric breakdown/3/, solidification of undercooled melts/4/, growth by electrochemical deposition/5/, precipitate growth in supersaturated systems/6/, and the flow through porous media/7/ have been investigated experimentally and theoretically. Recently it has been shown, that a special class of dendritic structures can represent stationary, stable states of an open system, and that these structures satisfy a variational principle. The aim of this paper is to illustrate, that the optimization of the corresponding quantity might be useful for living beings.

2 Dendritic patterns which satisfy a variational principle

One of the simplest physical systems that generates optimal dendritic patterns has been presented by Georgii et al./8/. The experimental set-up essentially consists of a cylindrical cell, made up by a 3 mm layer of castor oil (because of its high dielectric constant) within an acrylic dish of 114 mm diameter and a 47 mm layer of air above. The inner perimeter of the dish is equipped with a grounded metal ring electrode. The potential between a metallic tip, at 47 mm above the center of the oil surface, and this ring is 20 kV. Charges are sprayed quasi homogenously upon the oil surface. The dish contains N metallic bearing balls, at first distributed randomly. Under the influence of the electric field they form a dendritic structure to transport the charges to the metal ring /9/. Since the layer of oil is thin, compared to the diameter of the cell, we use a two dimensional model and investigate the electric field between the balls. The potential energy W results from

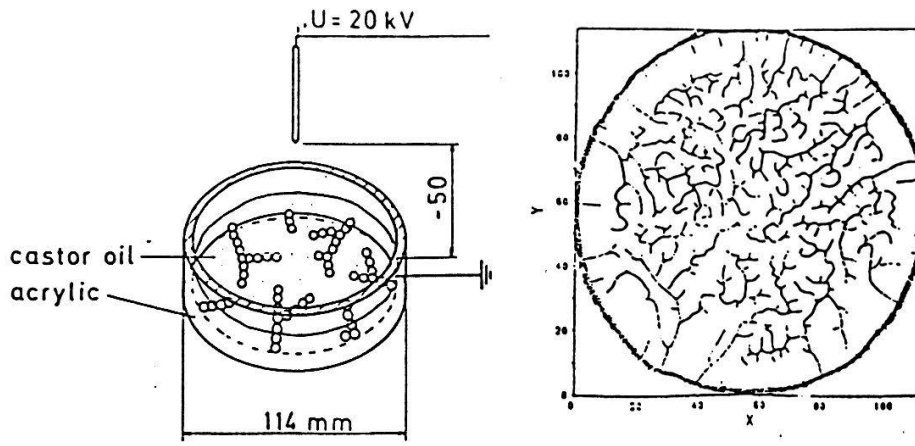


Figure 1: a) Experimental set-up b) Picture of a dendrite

$$W = \int_{oil} \epsilon (\nabla \Phi)^2 d\vec{x} \quad (1)$$

where ϵ is the dielectric constant of the oil and the electric potential Φ is calculated from

$$\sigma \Delta \Phi(\vec{x}, t) = S(\vec{x}, t) + \frac{\partial \rho(\vec{x}, t)}{\partial t} \quad (2)$$

$\vec{x}$ and t are position and time respectively. The conductivity of the oil is σ , ρ is the charge density at the surface and S counts the number of charges which are sprayed, per unit time, onto the surface at position $\vec{x}$. To derive equation (2) the continuity equation for the charges has been used under the constrain that Ohm's law is valid. The source of charges S of equation (2) is assumed to be constant. The metallic balls, which are assumed to be ideal conductors, are represented by small circular areas centered around position $\vec{q}_i (i = 1, 2, \dots, N)$. We assume further that the dynamics of the balls can be modelled by

$$\gamma \dot{\vec{q}}_i = - \nabla_{\vec{q}_i} W \quad (3)$$

in which γ is the friction constant. If the electrical relaxation time of equation (2) is very small compared to the mechanical relaxation time resulting from equation (3), in addition to the boundary conditions the electric potential $\Phi(\vec{x}, t, \vec{q}_i(t))$ is a function of $\vec{x}$ and of the positions $\vec{q}_i$ of the balls only. If the boundary conditions for the current are kept fixed, the electric potential Φ is slaved /9/ by the positions $\vec{q}_i$ of the balls, i.e. $\Phi = \Phi(\vec{x}, \vec{q}_i(t))$. In this case W is a Lyapunov function of the system. Therefore the local and global minima of W are stable stationary states /9/. Since the dissipation P is proportional to the potential energy W , the system approaches a state with minimal dissipation, i.e. a minimal production of heat. It has recently been shown experimentally that the geometry of the stable patterns satisfies the scaling relations

$$W \sim M^{-D_M} \quad (4)$$

$$W \sim N^{-D_N} \quad (5)$$

where D_M and D_N are dependent on the geometry of the experiment and of the current traversing the system. M is the number of the tips of the structure and N is the number

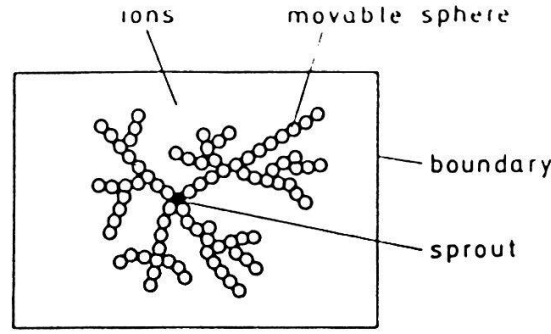


Figure 2: Modell of a root system

of directly or indirectly grounded balls, D_M and D_N are independent of M or N . Further *Merté et al./9/* have shown that the optimal patterns are ramified and simply connected. Obviously these are some of the properties of plants. In the following chapter we will present a mathematical link between the properties of roots and the optimal dendritic structures of the physical system.

3 Optimal structures for roots

The purpose of the root system of plants is the mechanical support of the plant as well as the absorbtion of ions and water. In the following we focus on the latter function and use a simplified, two dimensional model of the root system (fig.2). The black dot in the center of the container represents the connection between the root system and the plant and is assumed to be an ideal absorber for ions. J quantifies the amount of ions which are homogenously spread into the container per unit time. N spheres are movable and represent the system of roots. Therefore we assume that the diffusion constant D_i for the ions inside the spheres is essentially higher than the diffusion constant D_s in the surrounding medium. Further we assume that ions can not diffuse across the boundary of the container. Due to these assumptions we have the following relation for the concentration ϱ of the ions

$$\frac{\partial \varrho(\vec{x}, t)}{\partial t} = D \nabla^2 \varrho(\vec{x}, t) + J \quad (6)$$

W_b is given by

$$W_b = \left| \int_{cell} (\nabla \varrho)^2 d\vec{x} \right| = \frac{J}{D_s} \bar{\varrho} \quad (7)$$

where $\bar{\varrho}$ is given by

$$\bar{\varrho} = \int_{cell} \varrho d\vec{x} \quad (8)$$

W_b depends on the positions of the balls and on J . If the pattern of spheres represents the stable state of the physical system of chapter 2, and J is constant, then W_b is minimal. A small value of W_b might be an advantage for the plant, if it competes with other plants, or other absorbers are in the surrounding medium. If we assume that a small value of W_b is an advantage for a plant, then we can conclude from chapter 2 that optimal root systems satisfy the following relation

$$W_b \sim M^{-D_M} \sim N^{-D_N} \quad (9)$$

M is the number of tips and N is the number of balls with direct or indirect contact to the black dot (the total mass of the root system). D_M and D_N are factors depending on the geometry of the experiment, as well as on the ion current traversing the system, and are independent of M.

4 Discussion

Of course the root system of real plants has to satisfy other properties too, e.g. resistivity against diseases. Since the root system of a huge variety of plants seems to be closely related to optimal physical dendrites, we assume that the optimization of W_b is an essential advantage for most plants. Since the basic equations which have been used in the physical system and the biological model are first order approximations for the general transport processes, the argument presented in this paper might be the basis for the explanation of the ramified systems of nerves (collection of information from the surroundings), arteries (distribution of oxygen etc.), and other dendritic structures in biological systems.

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+ part of Ph.D. thesis

MRI Water-Fat Classification by Differential
Phase and Phase Correlation

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Abstract

When using a chemical-shift to separate the water and the fat protons in a Magnetic Resonance Imaging sequence, it is desirable to characterize each pixel by its phase and to assign to each pixel in the image a color or gray level according to the chemical species to which it belongs.

We propose two approaches to classify the pixels based on algorithms which compare the angle of the surrounding pixels. The first algorithm assumes that a small change is due to local perturbations and bigger jumps account for a change in the proton species. The second assumes that the amount of pixel-to-pixel change is indicative of the species.

Theory

The magnetic resonance signal induced by the precessing magnetic moment of the protons has a frequency given by the Larmor equation: $\omega_0 = \gamma B_0$ where γ is the gyromagnetic ratio for the proton and B_0 the static magnetic field. Due to the chemical shift effect, the Larmor frequency changes slightly depending on the molecule or the location of the proton in the molecule¹⁾.

As Magnetic Resonance Imaging is mainly used in medicine, the protons in water and in lipids constitute the vast majority of the protons present in the biological tissues, accounting for about 40% of the organic matter in the body. The lipids are essentially triacylglycerols (triglycerides) and are generally referred to simply as fat. A typical spectrum obtained from animal or human tissue is shown in figure 1 where the larger signal is water and the smaller is due to the CH_2 group of fat. The two peaks are 3.5 ppm apart.

For now, let us restrict the discussion to just one pixel (voxel) which we assume contains the same amount of protons in each species (H_2O and CH_2) having respectively the frequencies ω_w and ω_f . We know that $\omega_w - \omega_f = 3.5$ ppm.

Immediately after the 90° saturation pulse²⁾ (time $t=0$), both signals are in phase, meaning they are along the OY

axis (or 0X). At that time the phase is zero ($\Phi=0$). Because of the 3.5 ppm difference between the two signals (224 Hz at 64 MHz), the two components will be in and out of phase with a period of 4.46 ms ($1/224$).

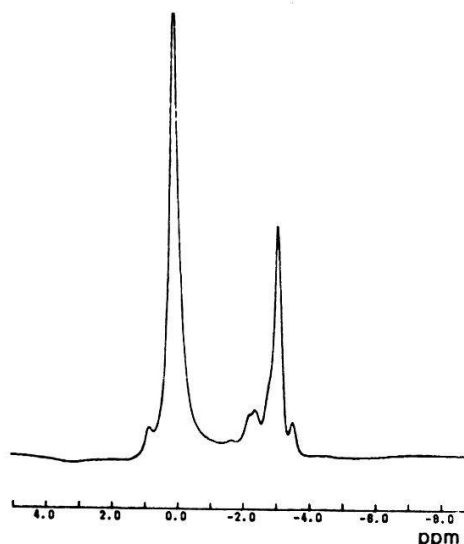


Figure 1

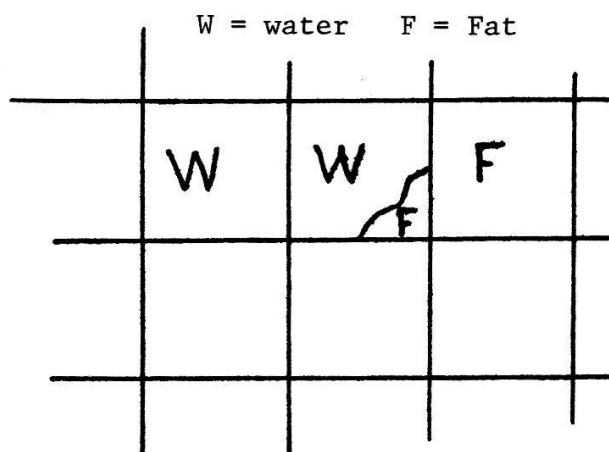


Figure 2

If we collect data at time $t=0$ or at any later time which is a multiple of 4.46 ms, the result will be the sum of the two contributing signals producing a maximum amplitude. On the other hand, if we collect the data at a time which is a multiple of 4.46 ms with the starting time at 2.23 ms, the two components are dephased by 180° and the amplitude is minimum³⁾.

The common design of an MR spectrometer uses quadrature detection in order to improve the sensitivity⁴⁾. Let us call the I-channel the one which is in phase ($\Phi=0$ at $t=0$) and the other one the Q-channel ($\Phi=90^\circ$). As shown in a previous paper²⁾, this special feature can be used to separate the two chemical species by shifting the 180° pulse by a time $\Delta\tau$.

In a standard spin-echo sequence, the echo occurs at time $TE=2\tau$ where it is assumed that the dephasing acquired during time τ is completely rephased during the second period of time τ . By collecting the data at time $TE + 2\Delta\tau$ or $TE - 2\Delta\tau$, we should sample the signals when they are separately rephased 90° apart.

In MRI, the standard SE sequence is tailored in such a way as to have the Hahn echo and the gradient echo formed at the same time. To achieve the water-fat separation, we manage to have the echoes occurring at different times, TE and TE + $2\Delta\tau$. In the method used here, $\Delta\tau$ is chosen in order to have the two signals dephased by 90° at the data acquisition time. The I-channel "sees" one chemical species and the Q-channel the other one. In other words, the I-channel is sampled when the Hahn echo (resulting from species A) is maximum and the Q-channel is sampled when the gradient echo (resulting from species B) is maximum.

We mentioned previously that every 4.46 ms the two signals are in phase. Consequently, to be 90° apart, the two echoes should occur separated by 1.05 ms. This is achieved by shifting the 180° pulse by $1.05/2 = .575$ ms.

The restriction to a single pixel made so far is unrealistic when applied to MRI. It turns out, due to the field inhomogeneities (B_0 and B_1), that the phase might vary from pixel to pixel preventing the simple quadrature classification to work. Even more worrisome is the fact that the expected 90° phase difference is not realistic when actual in vivo experiments are performed because each adipose containing pixel is a mixture of water and fat (see figure 2).

Pixel by pixel classification

Since the phase from one pixel to its neighbor should be identical if they contain the same chemical species, and the phase makes a big jump if the species changes, we should be able to correctly classify each pixel using this differential and given a known starting pixel. There remains some uncertainty if we are looking at a pixel occurring at the boundary of the two substances, but this may be overcome by looking at a larger neighborhood.

To test the method, a piece of fatty beef was used. Initially, a phantom containing oil and water was tried, but

this produced artificially good results and did not mimic the water-fat distribution in the human body. The differential classification described was applied to the meat and did not give encouraging results. This is mainly due to noise at edges and the relatively large deviation of the amount of water in intra-abdominal fat regions.

A second classification scheme using what we call the phase activity was then tried. This method classifies according to the pixel-to-pixel deviation in phase. A region of large deviations is classified as fat, otherwise as water. Although there are problems to overcome with this method as well as more statistical and biological analysis, results are promising. Figure 3a shows the actual repartition of fat and muscle and figure 3b is the MRI classified image.



Figure 3a

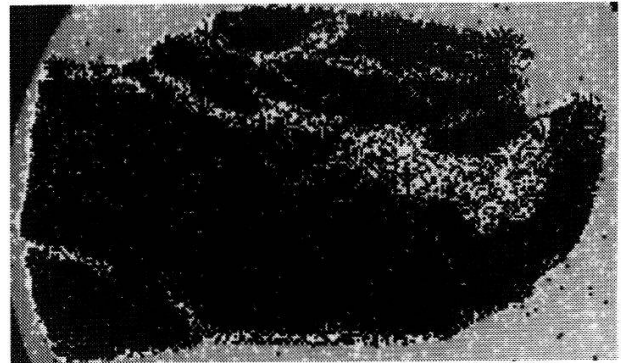


Figure 3b

As seen on the above images, fairly good agreement is achieved between what is recognized as fat in the picture and what is actually classified as fat.

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STRUCTURAL CHARACTERIZATION OF ULTRA-SHORT PERIOD
Si-Ge SUPERLATTICES

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Abstract: We present Rutherford Backscattering (RBS) and channeling studies obtained on ultra-short period Si-Ge superlattices (SL's) grown on $\text{Si}_{1-x}\text{Ge}_x/\text{Si}(100)$. From X-ray scattering SL periodicities down to 8 monolayers have unambiguously been confirmed. Moreover, a combination of RBS and X-ray results yields the strain distribution in the SL's. Pseudomorphic growth up to several thousand Å has been achieved on buffer layers with intermediate composition ($x \sim 0.5$).

1. Introduction

Strained-layer Si/Ge heterostructures, grown epitaxially on Si, have been playing an ever increasing role in the past few years. Most of the work has been done on strained $\text{Si}_{1-x}\text{Ge}_x$ alloys and $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ superlattices [1]. But only recently, reports on new optical transitions in short period superlattices consisting of pure Si and pure Ge layers [2] (Si_nGe_m SL's) have greatly stimulated the activities of experimentalists and theorists in the field. In addition, the nature of the lowest electronic transitions has been shown to depend strongly on the lattice constant to which the SL is strained, i.e. the substrate [3,4]. A most promising perspective concerning these thin layer Si_nGe_m SL's is the predicted existence of a nearly direct fundamental bandgap.

2. Experimental

We use 3 inch diameter, (100)-oriented and phosphorus doped ($0.05 - 5.0 \Omega\text{cm}$) Si wafer as substrates. They are cleaned thermally by heating to 830 °C for ~30 min and subjecting them to a small Si flux (total amount of deposited Si: ~10 Å). Subsequently a

Si-buffer of 500 - 1000 Å is grown. The substrates prepared in this manner exhibit a smooth surface, with a $2 \times 1 + 1 \times 2$ RHEED pattern. The silicon is evaporated from an electron gun, the germanium from a Knudsen cell. The growth rate for Si is monitored by a quartz crystal balance, the dependence of the Ge rate on the Knudsen cell temperature has been calibrated by RBS. The base pressure in our MBE machine is 10^{-11} mbar, not exceeding 10^{-9} mbar during growth.

RBS spectroscopy and channeling are known to be an excellent tool not only to measure the thickness and the stoichiometry of thin films, but also to probe their structural perfection. Channeling spectra are taken by aligning the beam along a major crystallographic direction. The minimum yield $\chi_{\min}$ which is the channeling yield normalized to the yield obtained with a random beam orientation, is a good means to describe the crystalline quality of a material. An ideal crystal has a $\chi_{\min}$ of about 3% [5].

3. Growth and Characterization

The greatest problem when growing thick epitaxial buffer layers onto Si is the suppression of 3-dim. growth. Since $\text{Si}_{1-x}\text{Ge}_x$ layers in general are lattice mismatched to Si (4% for pure Ge), there is a critical thickness H_c for pseudomorphic growth, the experimental values for which can be found in refs. 6 and 7. For intermediate compositions ($x \sim 0.5$), H_c is in the order of 120 Å. Extending the thickness beyond H_c results in the generation of misfit dislocations, which may act as nucleation centers for 3-dim. growth. In order to ensure a 2-dim. growth mode and thus smooth surfaces, we keep the substrate temperature T_s as low as 420 °C for the initial stage of growth. In addition, we use a relatively high growth rate of ~ 2 Å/s. After some hundreds of Å, T_s can be raised in steps up to 550 °C. It has also been found that the morphology depends strongly on the Ge content in the buffer and for Ge compositions of 30 - 70%, 2-dim. growth is difficult to achieve [8]. After ~ 2000 Å, we had to lower T_s again below 520 °C to prevent deterioration of the surface. Fig. 1 shows a 5500 Å thick $\text{Si}_{1.5}\text{Ge}_{0.5}$ alloy buffer layer on Si(100). As can be seen from the high $\chi_{\min}$ ($\sim 50\%$) near the Si/alloy interface, the layer is of minor crystalline quality in this region due to the generation of misfit dis-

locations. Towards the surface, however, the channeling yield decreases down to 6.1%.

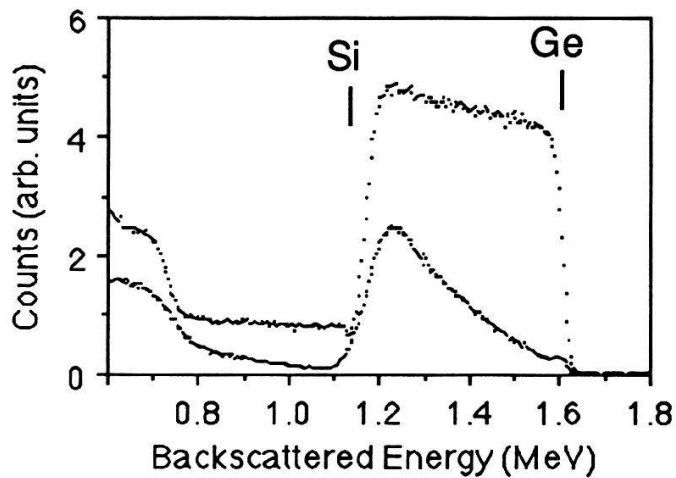


Fig. 1: <110> channeling and random spectra from a 5500 Å alloy buffer layer ($x=0.5$)

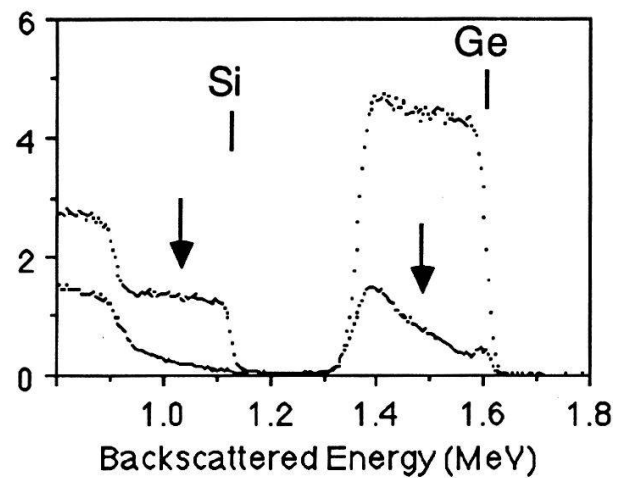


Fig. 2: <110> channeling and random spectra from a 1600 Å Si_6Ge_4 SL on a 2000 Å buffer

Si_nGe_m superlattices grown onto a $\text{Si}_{1-x}\text{Ge}_x$ alloy buffer of the same composition have the great advantage, that they are lattice matched as a whole. In other words, the SL's are symmetrically strained, the Si and Ge layers being dilated and compressed, respectively [9]. As a result, there is no thickness limitation for pseudomorphic growth for this type of SL, as long as the individual Si and Ge layers themselves are below their critical thickness. We have grown short period SL's consisting of 4/4, 5/5 and 6/4 monolayers of Si and Ge, respectively, onto alloy buffer layers of the appropriate composition. The growth temperature has been 400 - 450 °C in order to maintain good morphology and the growth rates ~ 1 Å/s for Ge and ~ 0.5 Å/s for Si. As an example, fig. 2 shows the random and channeling spectra of a Si_6Ge_4 SL (116 periods, total thickness: 1600 Å) on top of a 2000 Å alloy buffer. Like in fig. 1, the alloy buffer starts with a relatively poor crystalline quality, but recovers to a $\chi_{\min}$ of 17% at the alloy/SL interface (marked by arrows in fig. 2). The superlattice itself has a reasonable quality of 8% at the surface. From X-ray diffraction yielding a single 0th order peak from superlattice and buffer, we can conclude that the

composite structure is relaxed to the average lattice constant of the free SL. The Si and Ge layers are thus under a strain of 1.7% and 2.3%, respectively.

In conclusion, we have found the temperature range for the growth of Si_nGem SL's to be highly limited due to the competitive requirements for good crystalline quality and 2-dim. growth. Despite the narrow range of growth temperature, optimizing the growth procedure and extending the thickness of the buffer layers should nevertheless make it possible to improve the crystalline quality of these short period Si_nGem SL's further.

4. Acknowledgement

We would like to thank very much Mr. H.-J. Gübeli for his excellent technical support and Dr. R. E. Pixley from the Physics Department of the University of Zürich for the opportunity to use his RBS equipment and the help therewith. Financial support of the Swiss National Science Foundation is also gratefully acknowledged.

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PARALLEL ELECTRIC TRANSPORT IN THIN CoSi_2 LAYERS ON $\text{Si}(111)$

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Abstract: We measured the parallel electric transport in ultra-thin (10 Å - 500 Å) epitaxial CoSi_2 layers. The layers were grown by coevaporation of Si and Co on a $\text{Si}(111)$ substrate held at room temperature. The silicide was formed by a subsequent in situ anneal between 350 °C - 650 °C. The dependence of the residual resistivity ρ_0 on the layer thicknesses is shown to behave in a way, which is not explained by classical theory. We have further investigated the manner in which the resistivity of the films depends on the annealing temperature. We would like to emphasize that all well annealed layers, even the thinnest ones (10 Å), show metallic behaviour.

Introduction

Thanks to the progress in crystal growth techniques in the last decade it has become possible to grow epitaxial metal layers on silicon [1,2]. Among these layers the metallic silicides are certainly the most examined group. CoSi_2 is not the representative with the best match to the silicon lattice (lattice mismatch 1.2%), but it has a low residual resistivity. Its electrical properties make it interesting specially for possible applications in future devices. That is why the growth of CoSi_2 on $\text{Si}(111)$ is studied by several groups all over the world [3,4,5]. The easiest and commonly used growth method is solid phase epitaxy (SPE). Thereby Co is electron gun evaporated on top of a clean Si substrate held at room temperature under ultra-high vacuum conditions. CoSi_2 is then formed by in situ annealing at typically 650 °C. This method has

several disadvantages, such as a visible roughness of the layers, even a milky shining surface when the final thickness exceeds 200 Å and finally a huge amount of pinholes in ultra-thin (<30 Å) films. We therefore suggested another technique which improved the morphology of the layers considerably. Details about the growth and structural characterizations have already been published elsewhere [5,6]. The method mainly consists of the coevaporation of Si and Co at an exactly stoichiometric ratio with the substrate held at room temperature. On annealing the formation of CoSi_2 takes place already at a temperature as low as 250 °C. But with a further anneal to 600 °C the structural and electrical properties of the films are improved, as can be seen in a decrease of the channeling yield in Rutherford backscattering experiments or an increase in the conduction of the films. It has to be noted however, that these properties are very sensitive to deviations from stoichiometry during the evaporation of Co and Si. This will be shown in the next paragraph. An important property of our films is the atomically sharp interface with silicon which can be seen in cross section transmission electron microscopy. The sharpness of the interface and the smooth surface on a macroscopic scale make our layers an ideal system to study physical properties as a function of layer thickness and to measure effects due to a reduced periodicity in the third dimension. The electrical transport should therefore be influenced by these effects.

Electrical Measurements

The measurements were made on structures defined by photolithography and mesa-etching. The configuration we used was a six-legged bridge enabling a four point measurement. The active areas were between 50 μm - 200 μm wide and 500 μm - 1000 μm long. Electrical contacts to the layers were made by ball point gold wire bonding. We could cool down the samples to 4 K using a liquid Helium tank as cryostat. In fig 1) is shown the residual resistivity ρ_0 of several different samples with different layer thicknesses. The bulk residual resistivity ρ_b (equal to 2.1 $\mu\Omega\text{cm}$) has been subtracted. The data shown correspond to the lowest possible ρ_0 's, attainable in most cases only after an anneal to 600 °C. This might

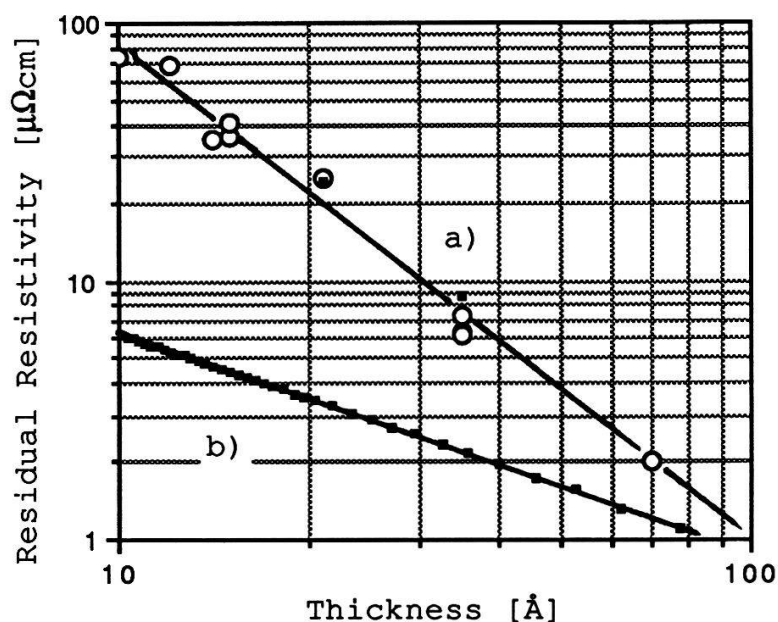


Fig. 1) Residual resistivity ρ_0 minus bulk resistivity ρ_b versus layer thickness

- a) measured data
- b) classical calculation with specularity parameter 0.9 [9].

be due to slight deviations from exact stoichiometry during the codeposition process. The values are lower than those previously reported [7,8] for films grown by SPE. The temperature dependence of the resistivity obeys Matthiessen's rule $\rho = \rho_0 + \rho_1(T)$, where $\rho_1(T)$ is due to scattering of electrons with phonons. For high T , $\rho_1(T)$ is linear in T and for small T it is proportional to T^x where $3 \leq x \leq 4$. Our films exhibit this temperature dependence, down to a thickness of 10 Å, i.e. they are all metallic. In particular, an increase in the resistivity at low temperatures due to weak localisation effects cannot be found on well annealed samples. The slope of $\rho(T)$ in the linear region has been found to depend on the annealing temperature, as does ρ_0 itself. Comparing samples with the lowest ρ_0 we find a slope which is nearly independent from the layer thickness (0.06-0.07 [$\mu\Omega\text{cm}/^\circ\text{C}$]). A more complete account of these findings will be given elsewhere. As has been noted by others [7,8] the rapid increase of ρ_0 with decreasing layer thickness d cannot be explained by classical theory, even when surface scattering is taken into account [9]. From fig. 1 we obtain $\rho_s = \rho_0 - \rho_b \sim d^{-1.9}$. To explain this behaviour the quantization of the electron k -vector perpendicular to the layer has to be taken into account. Surface roughness on an atomic scale leads to a variation of the number of occupied subbands across the layers. Intersubband scattering is then expected to play a major role in the parallel elec-

tric transport. The quantum mechanical theory of Fishman and Calecki [10] can quantitatively explain the observed behaviour. To fit their theory to data similar to the present ones, they had to introduce a mean roughness amplitude of 4 Å with a correlation length of 2 Å. In particular the latter value seems somewhat unphysical, however.

In conclusion we have shown that the codeposition technique together with an appropriate annealing procedure leads to epitaxial CoSi_2 - films with excellent metallic properties down to thicknesses of a few monolayers.

Acknowledgement

We express our deep gratitude to Mr. H.J. Gübeli for his technical assistance. Financial support by the Swiss National Foundation (NFP 19) is gratefully acknowledged.

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BaF₂-SrF₂-CaF₂(100) LAYERS ON Si(100) WITH SMOOTH SURFACES

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Abstract

Epitaxial BaF₂ layers have been grown by molecular beam epitaxy (MBE) onto Si(100). Despite the large lattice mismatch of 14% and preferred (111)-growth mode, (100)-oriented BaF₂ layers were obtained if a thin intermediate CaF₂, SrF₂ or CaF₂-SrF₂ layer was deposited first. Rutherford backscattering minimum channeling yields of 3.5% for layers of a thickness of 4000 Å only indicate a considerable structural quality. Although nucleation is 3-dimensional, perfectly smooth layers can be obtained by choosing proper growth temperatures. The results indicate that the high free energy of the (100)-surface of the fluorides is reduced to less than $\sqrt{3}$ times the (111)-surface free energy at high enough temperatures, thus allowing 2-dimensional growth of (100)-oriented fluoride layers in a certain temperature range. The layers are intended for use as buffers for heteroepitaxy of heavily lattice-mismatched II-VI and IV-VI compound semiconductors on Si.

Introduction

With regard to heteroepitaxy on Si substrates, group IIa fluorides received considerable attention. Most work has been performed with Si/CaF₂ structures where the lattice mismatch is 0.6% at room temperature [1-5]. For epitaxial growth of highly lattice mismatched semiconductors like CdTe, HgCdTe or PbTe (=19% to Si) we need fluoride combinations like SrF₂/Si (mismatch 7%) or BaF₂/Si (mismatch 14%). If a thin (=100Å) CaF₂ or SrF₂ layer is grown first, BaF₂ can be grown quite easily and with good quality on Si(111) [6]. Such stacked fluoride layers have been applied as epitaxial buffers to grow for the first time epitaxial narrow-gap IV-VI semiconductors on Si for infrared sensor array applications [7-9] as well as epitaxial CdTe on Si(111) [10].

Since (100)-surfaces are preferred in Si device technology, buffers on Si(100) containing BaF₂ top layers would allow the growth of heavily lattice-mismatched compound semiconductors on (100)-oriented wafers. While CaF₂ grows with the same (100)-lattice orientation as Si, it was found in early work [1] that the highly mismatched SrF₂ and BaF₂ grown on Si(100)-surfaces align their [111]-direction perpendicular to the surface, and consist of multiply-orientated crystallites with rather poor structural quality.

It is more difficult to grow fluoride layers with (100)- than with (111)-orientation as the low (111)-surface free energy of fluorides leads to a preferred (111)-growth mode. If one tries to calculate the free energy of the perfect (100)-surface, the corresponding Madelung sum diverges [2]. It was found that CaF₂ can be grown epitaxially on Si(100) in a narrow substrate temperature range around 550°C only [1]. Nucleation is 3-dimensional as revealed by spots in reflection high-energy electron diffraction (RHEED) patterns. The surface of even thick layers consists of a dense array of pyramids with (111) side faces and around 200 Å basal widths [2,5]. However, flat CaF₂ surfaces showing corresponding streaks in the RHEED-patterns have been obtained recently using either a two-temperatures step growth with the substrate temperature increased to >800°C after growth of the first layer about 400 Å thick [4], or by in-situ annealing at at least 900°C. This flattening of the surface was determined to be due to surface diffusion.

In this contribution, we discuss our results of BaF_2 growth on $\text{Si}(100)$. Intermediate thin CaF_2 and/or SrF_2 layers were used in order to surmount the high lattice mismatch in a stepwise manner and to achieve (100)-epitaxy.

Experimental

We have grown the layers in a MBE apparatus equipped with RHEED and AUGER facilities. The substrates were heated by direct thermal radiation incident on the back sides of the wafers. The background pressure during growth was in the 10^{-9} mbar range and growth rates were about 0.1 – 0.3 nm/s. The wafers were cleaned with the Shiraki method and heated in situ until the well known 2×1 surface reconstruction appeared. Carbon contamination was below 0.01 monolayer after this step. In all cases, layers of CaF_2 and/or SrF_2 (100 – 150 Å thick) were deposited first, followed by BaF_2 of a thickness of 2000 – 5000 Å, and all layers described below were (100)-oriented.

Results and discussion

If the whole growth of the multilayers was performed at 560°C [the temperature considered to be optimal for initial condensation of CaF_2 on $\text{Si}(100)$], the resulting BaF_2 surface appeared smooth in the optical microscope, but some roughness was revealed with scanning electron microscopy (SEM). This roughness is on a 100 nm scale for a SrF_2 - CaF_2 intermediate buffer layer as shown in Fig. 2, or somewhat rougher for a single CaF_2 intermediate buffer and slightly altered growth conditions [11]. However, the RBS minimum channeling yield is 3.5%, as low as for bulk BaF_2 or (111)-oriented epitaxial BaF_2 layers on $\text{Si}(111)$ [6,7], indicative of a good crystalline quality.

To demonstrate the effect of a two-temperatures growth method, we first deposited SrF_2 (≈ 150 Å) at 560°C substrate temperature. Spotty RHEED patterns were observed as expected, but some rings due to misoriented grains also sometimes formed. After a short in situ anneal cycle (10 s at 950°C) the rings disappeared and the RHEED pattern became spotty with weak streaks joining the spots. The streaks are due to islands with elongated (111)-facets as described elsewhere [12]. BaF_2 growth was then started at $\approx 580^\circ\text{C}$, and after deposition of about 400 Å of BaF_2 , the second growth step was initiated by increasing the substrate temperature to above 800°C. The total thickness of the BaF_2 layer was about 4500 Å. A considerable crystalline quality of this layer is indicated by a RBS minimum channeling yield of $\approx 4\%$ (Fig. 3). Fig. 4 shows a micrograph of the structure. The surface is partly covered with truncated pyramids, but perfectly smooth on their top faces and between them, at least as far as discernible with the SEM technique. The main part of this layer exhibits a (100)-surface. The surface morphology is the same as for CaF_2 on $\text{Si}(100)$ under certain growth conditions [4].

As in the case of $\text{BaF}_2(111)$ -layers on $\text{Si}(111)$ [6], no cracks were detected in all these BaF_2 -terminated layers because thermal mismatch strain relieves by some plastic deformation [11].

Growth model

The present results together with earlier work [1–5] suggest the following growth model of group IIa fluorides on (100)-oriented substrates.

The start of CaF_2 (or SrF_2) growth on $\text{Si}(100)$ is possible in a narrow temperature range around 550°C only. Growth is by 3-d nucleation. The nuclei form (111)-faces resulting in islands with a pyramidal shape with four (111) faces. The approximate spacing of the islands is ≈ 200 Å [2,5]. The same spacing is also observed for $(\text{Ca},\text{Sr})\text{F}_2$ on $\text{GaAs}(100)$ - [13] and $(\text{Sr},\text{Ba})\text{F}_2$ on $\text{InAs}(100)$ -layers [14], indicative of a similar nucleation of near lattice matched IIa fluorides on polar as well as on nonpolar semiconductors.

When the islands have grown together after a mean layer thickness of ≈ 45 Å (determined by the island shape and spacing) is reached, the surface remains faceted due to the preferred (111)-growth mode and little surface diffusion. However, if the substrate temperature is increased after this stage of growth, it is possible to obtain layers with a true smooth (100)-surface. Therefore, either the surface diffusivity increases considerably with temperature, rounding all edges in the layer until (111) faceting can no longer be observed, or the energy of the (100)-surface becomes smaller than that of the (111)-surface above a certain temperature. This temperature must lie above or around 700°C , as Asano et.al. [5] were able to grow smooth CaF_2 layers on flattened CaF_2 substrates at temperatures higher than 700°C , but not at 600°C . From this, we conclude that the (100)-surface free energy is lower than $\sqrt{3}$ times the (111)-surface free energy, as the total surface area of a closely spaced, regularly arranged array of (111)-sided pyramids with (100)-basal planes is $\sqrt{3}$ times higher than that of the corresponding flat (100)-basal plane. The truncated pyramids of Fig. 4 are due to incomplete surface flattening with the growth conditions indicated above, and could be completely avoided by a proper adjustment of the growth rate or substrate temperature during growth.

We conclude that the real (100)-surface of group IIa fluorides has a considerable different structure compared to the ideal case. While the calculated (100)-surface energy would be infinite, the actual values must lie below $\sqrt{3}$ times that of the (111)-surface (≈ 350 ergs cm^{-2} for BaF_2 , ≈ 480 ergs cm^{-2} for CaF_2 [15]). Further work is needed in order to clarify the actual (100)-surface structure of these fluoride layers.

Acknowledgements: The authors would like to thank P. Waegli, ETH Zürich, for performing the SEM investigations, Prof. V. Meyer and Dr. R. Pixley, University of Zürich, for the kind permission and help in using their Van-de-Graaff apparatus for the RBS investigations, and Prof. G. Kostorz, Institute of Applied Physics, ETH Zürich, for valuable discussions. The work is sponsored by the Swiss National Science Foundation.

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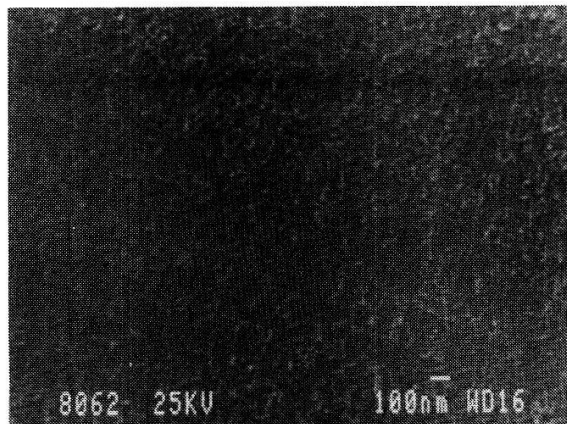
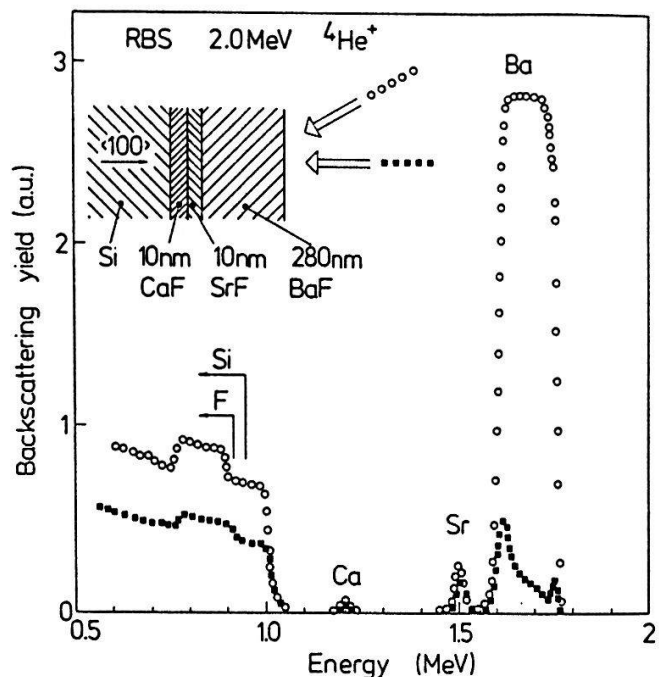


Fig. 1. RBS random and aligned spectra of a Si(100)/CaF₂-SrF₂-BaF₂ stack grown at 560°C with minimum channeling yield as low as 3.5%.

Fig. 2. SEM micrograph of the sample of Fig. 1 with a slightly rough surface.

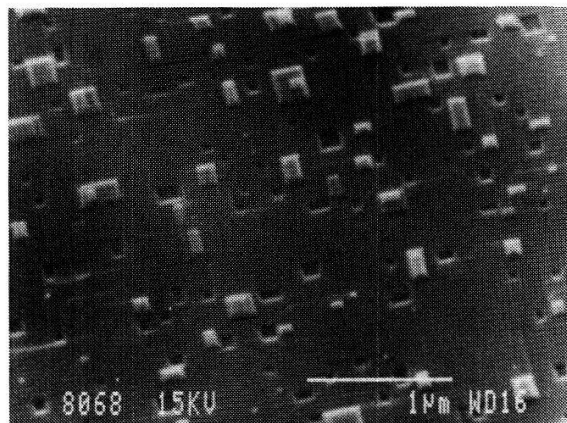
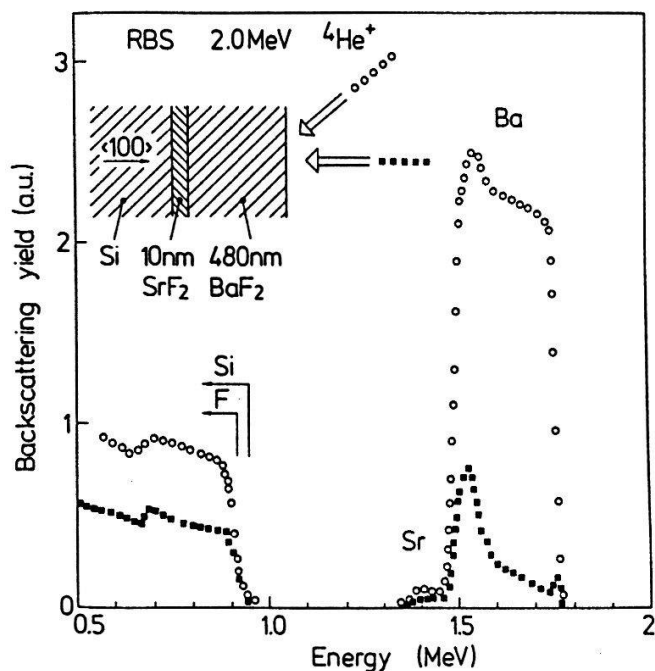


Fig. 3. RBS random and aligned spectra of a Si(100)/SrF₂-BaF₂ stack grown with a 2-temperatures method, showing minimum channeling yield of 4%.

Fig. 4. SEM micrograph of the sample of Fig. 3 showing structureless (100)-surfaces on top and between the truncated pyramids.

Photovoltaische Infrarotsensoren auf Silizium Substraten

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Zusammenfassung:

Aus 66 Elementen bestehende bilineare photovoltaische Infrarotsensor-Arrays wurden in heteroepitaktisch auf Silizium gewachsenen PbTe-Schichten gefertigt.

Durch einen Blei-Schottkykontakt wurde auf dem p-leitenden PbTe ein bis zu einer Grenzwellenlänge von 5.6 μm infrarotempfindlicher Sensor gebildet. Das Widerstandsflächenprodukt bei 85K ohne Vorspannung beträgt bis zu 2000 Ωcm^2 . Seine Temperaturabhängigkeit zeigt unterhalb von 115K verarmungszonen-limitiertes Rauschverhalten, während darüber die theoretische Diffusions-rauschgrenze erreicht wird. Unter 130K dominiert das Rauschen der Raumtemperaturstrahlung.

Einleitung:

Infrarotsensoren aus Schmalbandhalbleitern wie die Blei-Chalkogenide sind wegen ihrem hohen Wirkungsgrad und der Möglichkeit ternäre Halbleiter mit variabler Bandlücke und damit mit variabler Grenzwellenlänge zu bilden für die Wärmestrahlungsdetektion bestens geeignet. Gegenüber anderen IR-Sensortypen (z.B. Silizide) können Schmalbandhalbleitersensoren wegen ihrem geringen Eigenrauschen bei höheren Temperaturen betrieben werden.

Die Signalverarbeitung, wie das Einlesen in ein CCD (Charge Coupled Device), kann nicht im Schmalbandhalbleiter selbst durchgeführt werden. Oft wird deshalb eine hybride Lösung gewählt, bei der ein die Signalverarbeitung enthaltender Siliziumchip mit dem Detektorchip verbunden wird [1]. Da für jedes Bildelement eine eigene elektrische Verbindung benötigt wird, ist sowohl die Anzahl Bildelemente wie deren Grösse stark beschränkt.

Eine elegantere Lösung besteht darin, den Schmalbandhalbleiter epitaktisch auf das Silizium aufzuwachsen. Dazu muss man sowohl die Gitterfehlpassung zwischen dem Silizium und dem Schmalbandhalbleiter wie auch die verschiedenen thermischen Ausdehnungen überwinden können. Dies geschieht mit einer

CaF₂-BaF₂ Zwischenschicht, die mit Molekularstrahlepitaxie (MBE) auf das Silizium aufgewachsen wird [2]. Die Infrarotdetektion findet dann im mit Heisswandepitaxie (HWE) aufgewachsenen Schmalbandhalbleiter statt, während die Signalverarbeitung im darunterliegenden Silizium erfolgt.

Frühere Arbeiten beschrieben Einzelsensoren, während hier ein bilinearer aus 66 Elementen bestehender photovoltaischer PbTe-Sensor-Array (Fig. 1) für das 3-5µm atmosphärische Fenster vorgestellt wird.

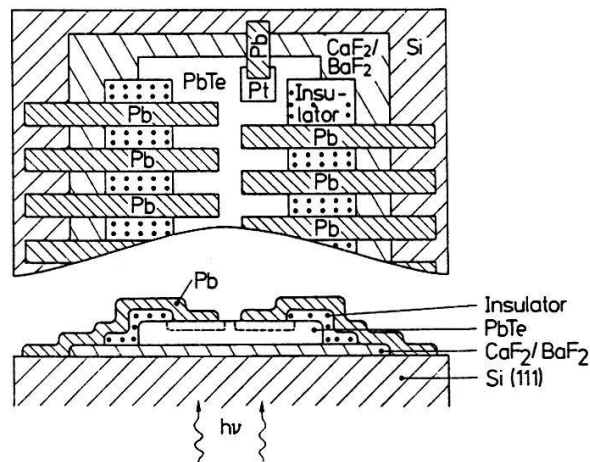


Fig. 1. Schematischer Aufbau des monolytischen bilinearen photovoltaischen IR-Sensorarrays. Die aktive Zone unter dem Blei-Schottkykontakt ist gestrichelt eingezeichnet.

Herstellungsprozess:

Mit MBE wird die 2000Å dicke Fluoridpufferschicht auf einen (111)-orientierten Si-Wafer aufgebracht [2].

Anschliessend wird das p-Typ PbTe in einer separaten HWE-Anlage aufgewachsen. Durch zusätzliches Verdampfen von Tellur wird die Löcherkonzentration von $4 \cdot 10^{17}/\text{cm}^3$ erreicht [3]. Die Wachstumsgeschwindigkeit beträgt ca. 3µm/h. Die Hallbeweglichkeit von 20'000 cm²/Vsek bei 80K ist mit der von auf massivem BaF₂ gewachsenen PbTe-Schichten vergleichbar.

Die aktiven Zonen des 66-elementigen Sensors werden durch Pb Schottkykontakte gebildet. Auf p-PbTe invertiert Pb die Oberfläche, so dass ein induzierter pn-Uebergang entsteht.

Als gemeinsamer ohmscher Kontakt dient aufgesputtertes Platin.

Charakterisierung:

Figur 2 zeigt die Strom-Spannungscharakteristik einer typischen Diode bei 90K. Der differentielle Widerstand im Nullpunkt beträgt 40MΩ, was einem Widerstandsflächenprodukt von 2000 Ωcm² entspricht.

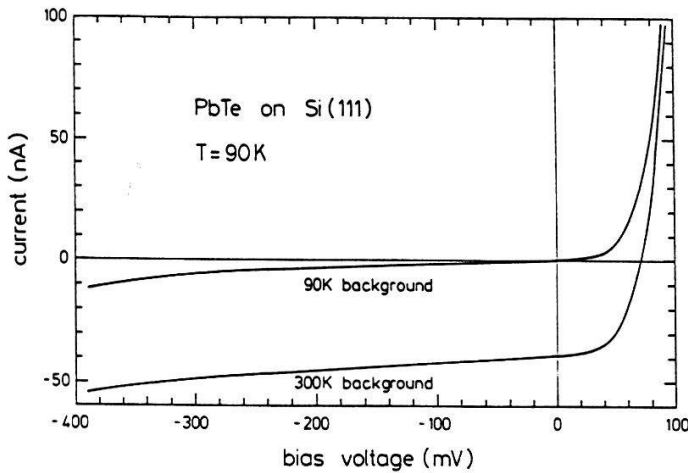


Fig. 2. Strom-Spannungscharakteristik einer typischen Diode bei 90K.

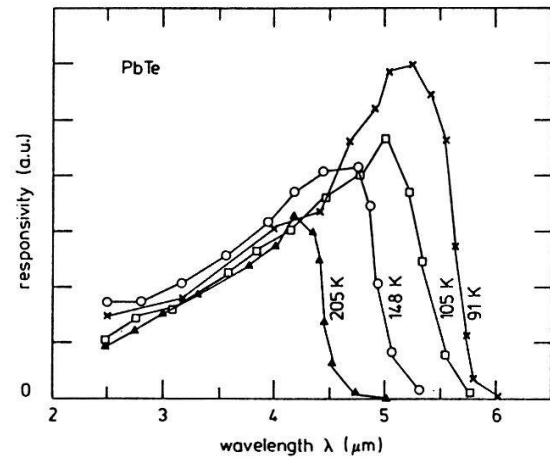


Fig. 3. Spektrale Empfindlichkeit (A/W) für ein PbTe Sensor bei verschiedenen Temperaturen.

Die spektrale Empfindlichkeit (Fig. 3) zeigt einen konstanten äusseren Quantenwirkungsgrad bis zur Grenzwellenlänge von $5.6\mu\text{m}$ bei 90K bzw. $4.4\mu\text{m}$ bei 205K. Die Verschiebung der Grenzwellenlänge zu kleineren Wellenlängen mit steigender Temperatur rührt von der positiven Temperaturabhängigkeit der Bandlücke her [4].

Der äussere Quantenwirkungsgrad ohne Antireflexionsschicht beträgt ca. 70%. Dies bedeutet, dass praktisch jedes Photon, das nicht reflektiert wird und damit die PbTe-Schicht erreicht, einen messbaren Photostrom erzeugt.

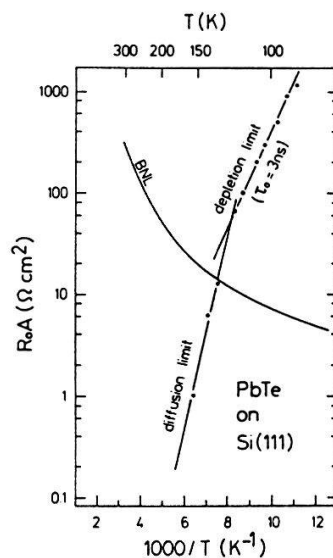


Fig. 4. Temperaturabhängigkeit des Widerstandsflächenproduktes eines PbTe IR-Sensors.

Die Temperaturabhängigkeit des Widerstandsflächenprodukts ohne Vorspannung (R_0A) einer typischen Diode ist in Figur 4 wiedergegeben. Für Temperaturen über 115K dominiert der Diffusionsdunkelstrom, der durch Auger Rekombination bestimmt ist, das Rauschen. $R_0A(T)$ ist dann proportional zu $\exp(E_g(0)/kT)$ [4].

Im verarmungszonenlimitierten Fall gilt [4]:

$$R_0A = \sqrt{\frac{E_g \cdot n_{ef}}{2 \cdot \epsilon_s}} \cdot \frac{1}{q \cdot n_i} \cdot \tau_0 \quad (1)$$

wobei ϵ_s die statische Dielektrizitätskonstante, n_{ef} die effektive- und n_i die intrinsische Ladungsträgerdichte, q die Elementarladung und τ_0 die Ladungsträgerlebensdauer für Shockley-Read Rekombination bezeichnet.

Aus (1) folgt, dass $R_0A(T)$ proportional zu $\exp(E_g(0)/2kT)$ ist. Die ausgezogene Linie in Fig. 4 entspricht Formel (1) mit $\tau_0 = 3\text{ns}$. Diese Lebensdauer ist genügend lang um Diffusion über mehrere μm bis zur Raumladungszone zu erlauben, wie es für das vollständige Einsammeln der photogenerierten Ladungsträger notwendig ist.

Weiter ist in Figur 4 das für hintergrundrauschbeschränkte Detektion (300K Hintergrund, 180° Blickwinkel, 70% Quantenwirkungsgrad) notwendige R_0A eingezeichnet. Unter 130K ist das Rauschen des Strahlungshintergrundes die dominierende Rauschquelle.

Ausblick:

Wir haben gezeigt, dass hintergrundrauschbeschränkte photovoltaische Blei-Chalkogenid IR-Sensorarrays produziert werden können. Der Herstellungsprozess ist mit standard Siliziumtechnologie kompatibel, so dass 2-dimensionale heteroepitaktische aber voll monolitische Infrarotsensoren hergestellt werden können.

Diese Arbeit wurde von der Gruppe für Rüstungsdienste (GRD) sowie von der europäischen Raumfahrtagentur (ESA) finanziell unterstützt.

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Refractive index change due the band-filling effect in GaAs/Al_xGa_{1-x}As phase modulators.

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Abstract: Using a parabolic density of state model, we demonstrate that the contribution due to band-filling in semiconductors optical phase modulators is proportional in first order to the carrier density and to the matrix element. Moreover, this contribution is independent on the carrier effective mass. This result is compared with numerical calculation and available experimental data.

1. Introduction

The doped double heterostructure optical phase modulator offers a high efficiency [1,2], and it is therefore a good candidate as an external phase modulator for high bit rate optical telecommunication systems. These structures are modulated by an electrical field which results in an refractive index change. This modulation is the sum of a linear electro-optic effect (or Pockel effect), a quadratic electrooptic effect and a term associated with the removal of carrier in the depletion zone [1,2,3]. This carrier contribution is the sum of a free carrier plasma term, a band filling and a many body effect term [3]. The aim of the paper is to compute analytically the band filling contribution using a parabolic band model.

2. Theory

The band filling effect is the refractive index difference associated with the Burstein shift of the absorption edge due to the removal of electron and holes from their respective bands. Let us consider a crystal of direct energy gap E_0 . Using parabolic bands and k (momentum) conservation, the absorption is the product of the joint density of state and of the difference between the Fermi distribution for the electron and holes[4]:

$$\alpha(E, E_F) = \frac{2^{5/2} e^2 \mu^{3/2}}{\hbar^2 n c m_0^2} \frac{\sqrt{E-E_0}}{E} |M|^2 (f_l - f_u) \quad (1)$$

where the Fermi distribution for the upper state f_u and lower state f_l are given by :

$$f_l = \frac{1}{1 + \exp\left[\frac{1}{kT} \left(-\frac{\mu}{m_h^*} (E-E_0) - E_F\right)\right]} \quad (2)$$

$$f_u = \frac{1}{1 + \exp\left[\frac{1}{kT} \left(E_0 + \frac{\mu}{m_e^*} (E-E_0) - E_F\right)\right]} \quad (3)$$

The origin of the energy is taken at the top of the valence band. μ is the reduce mass and $|M|$ the momentum matrix element. As $E_0 \gg kT$, the Fermi level is close to the conduction band and therefore $f_l \cong 1$. When the crystal is depleted, the Fermi level is close to center of the gap and in this case we have $f_u \cong 1, f_l \cong 0$. The case of holes is treated symmetrically, inverting m_e^* and m_h^* in the equations (2) and (3), and inverting the positive energy direction and taking the origin at the bottom of the conduction band. The absorbtion difference (crystal with carriers minus crystal depleted) is given by:

$$\Delta\alpha(E, E_F) = \frac{2^{5/2} e^2 \mu^{3/2}}{\hbar^2 n c m_0^2} \frac{\sqrt{E-E_0}}{E} |M|^2 f_u \quad (4)$$

In order to obtain the refractive index difference, we use the Kramer-Krönig integral [5]:

$$\Delta n(E) = \frac{\hbar c}{\pi} P \int_0^\infty \frac{\Delta\alpha(E)}{(E^2 - E_0^2)} dE \quad (5)$$

Intruducing equation (4) in (5) gives:

$$\Delta n(E_1, E_F) = \frac{\hbar c}{\pi} \frac{2^{5/2} e^2 \mu^{3/2}}{\hbar^2 n c m_0^2} P \int_{E_0}^\infty \frac{\sqrt{E-E_0}}{E (E^2 - E_1^2)} \frac{1}{1 + \exp\left[\frac{1}{kT} \left(E_0 + \frac{\mu}{m_e^*} (E-E_0) - E_F\right)\right]} dE \quad (6)$$

As we have $E_1 < E_0$ (the energy at which the refractive index variation is computed is sufficiently far from the energy gap), the term $E (E^2 - E_1^2)$ is slowly varying and is taken outside the integral:

$$\Delta n(E_1, E_F) = \frac{2^{5/2} e^2 \mu^{3/2}}{\hbar n \pi m_0^2} \frac{|M|^2}{E (E^2 - E_1^2)} P \int_{E_0}^\infty \frac{\sqrt{E-E_0}}{1 + \exp\left[\frac{1}{kT} \left(E_0 + \frac{\mu}{m_e^*} (E-E_0) - E_F\right)\right]} dE. \quad (7)$$

By making the substitution $x = \frac{\mu}{m_e kT} (E - E_0)$, we recognise in the right hand side of equation (7) the Fermi integral relating the Fermi level to the carrier concentration:

$$n_e = \frac{1}{2\pi^2} \left(\frac{2 m_e^*}{\hbar^2} \right)^{3/2} \int_{E_0}^{\infty} \frac{\sqrt{E - E_0}}{1 + \exp\left(\frac{E - E_F}{kT}\right)} dE \quad (8)$$

Inserting equation (8) into equation (7), we finally obtain:

$$\Delta n(E_1) = \frac{4 \hbar^2 e^2 |M|^2 \pi}{n m_0^2 \bar{E} (\bar{E}^2 - E_1^2)} n_{e;h} \quad (9)$$

2. Discussion

An appropriate value for $\bar{E}$ is $\bar{E} = E_0 + kT$. This result is only valid when E_1 is sufficiently far from E_0 (in kT units). However, this result requires no approximation in the Fermi integral calculation as this integration is implicit. It is very interesting to note that equation (9) does not depend on the electron or hole effective mass, and therefore the refractive index difference is the same for electron and holes. The numerical calculation given in [3], using exactly the same parabolic band model, are in total contradiction with this result as they predict a refractive index difference five times smaller for the holes than for the electrons. $|M|$ is often deduced from absorption measurements. Equation (9) is thus rewritten as:

$$\alpha(E) = \Phi_0 \frac{\sqrt{E - E_0}}{E} \quad (10a)$$

$$\Delta n(E_1) = \Phi_0 \frac{4 \hbar^4 c \pi}{2^{5/2} \mu^{3/2}} \frac{n_{e;h}}{\bar{E} (\bar{E}^2 - E_1^2)} \quad (10b)$$

In the case of GaAs, we impose the absorption at 1.6 eV to be equal to Casey's value $\alpha = 1.74 \cdot 10^4 \text{ cm}^{-1}$ [6]. This implies $\Phi_0 = 64 \cdot 10^3 \text{ cm}^{-1} (\text{eV})^{1/2}$, and equation (10b) has numerical values:

$$\Delta n(E_1) = 4.16 \cdot 10^{-21} \frac{n_{e;h}}{\bar{E} (\bar{E}^2 - E_1^2)} \quad (10c)$$

We compare this result with the refractive index measurements performed by Henry [7] on a buried double heterostructure GaAs laser. In this experiment, the refractive index difference is obtained by a Kramers-Krönig

the refractive index difference is obtained by a Kramers-Krönig transformation on the measured absorption spectra, and thus include only the band-filling and band shrinkage effect. At an energy $E=1.24\text{eV}$, Henry's result exhibit a linear relationship between the refractive index difference and the carrier concentration [8]:

$$\Delta n = - 6.1 \cdot 10^{-21} (\Delta n_e + \Delta n_h) \quad (2.46)$$

The measurement is made under current injection, and the neutrality is preserved ($\Delta n_e = \Delta n_h$). At this energy, equation (10c) gives a prefactor of $10.2 \cdot 10^{-21} \text{cm}^3$ instead of $6.1 \cdot 10^{-21} \text{cm}^3$. We attribute the difference between these two values to many body effects such as band shrinkage and band tailing.

4. Conclusion

Using a one electron parabolic band model, we demonstrate that the refractive index difference due to the band filling effect in direct bandgap semiconductors is proportional to the carrier concentration and independent of the carrier effective mass. This result is demonstrated for energies several kT below the energy gap. Comparison of this result with experimental data show that many body effect such as band shrinkage cannot be neglected [9].

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Photoluminescence of disordered $GaAs/Al_xGa_{1-x}As$ Quantum Wells via Zinc Diffusion

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Abstract: Zinc diffusion on multi quantum well structures was carried out. The impurity induced disordering depth was estimated by scanning electron microscopy. The concentration of aluminium in the disordered alloy was determined by low temperature photoluminescence (PL). A discussion of the PL spectra gives some insight for the mechanism of the Zinc induced disordering.

1. Introduction

Quantum well structures can be destroyed by the diffusion of impurities [1]. The impurities enhance the intermixing of the host crystal atoms, so that the quantum well layers become disordered [2]. Up to now, Zn diffusion-enhanced intermixing of $Ga - Al$ atoms in $GaAs/Al_xGa_{1-x}As$ structures has been most extensively studied [3]. At $600^\circ C$ the observed impurity enhanced diffusivities of Ga and Al are higher about 10^5 than their interdiffusivity at $800^\circ C$ [2].

In this contribution we study the photoluminescence (PL) of Zn diffused and impurity induced disordered Multi Quantum Well (MQW) sample. The impurity disordering depth was determined by Scanning Electron Microscopy (SEM). The low temperature PL yields informations about the electronic states of the disordered structure [4].

2. Experiment

The MQW sample was grown by MBE at a substrate temperature of $600^\circ C$ and consisted of $0.2 \mu m$ of $GaAs$ followed by a $1 \mu m$ thick buffer layer of $Al_{0.3}Ga_{0.7}As$ and 35 QW formed of $300 \text{ \AA}$ of $GaAs$ wells and $100 \text{ \AA}$ of $Al_{0.3}Ga_{0.7}As$ barriers. The terminating layer was $300 \text{ \AA}$ of $GaAs$. Figure 1 show the PL spectrum (part a) and the SEM photograph (part b) of the sample. In Fig. 1(a) we note the light hole exciton X_{lh} (1.5246 eV), the

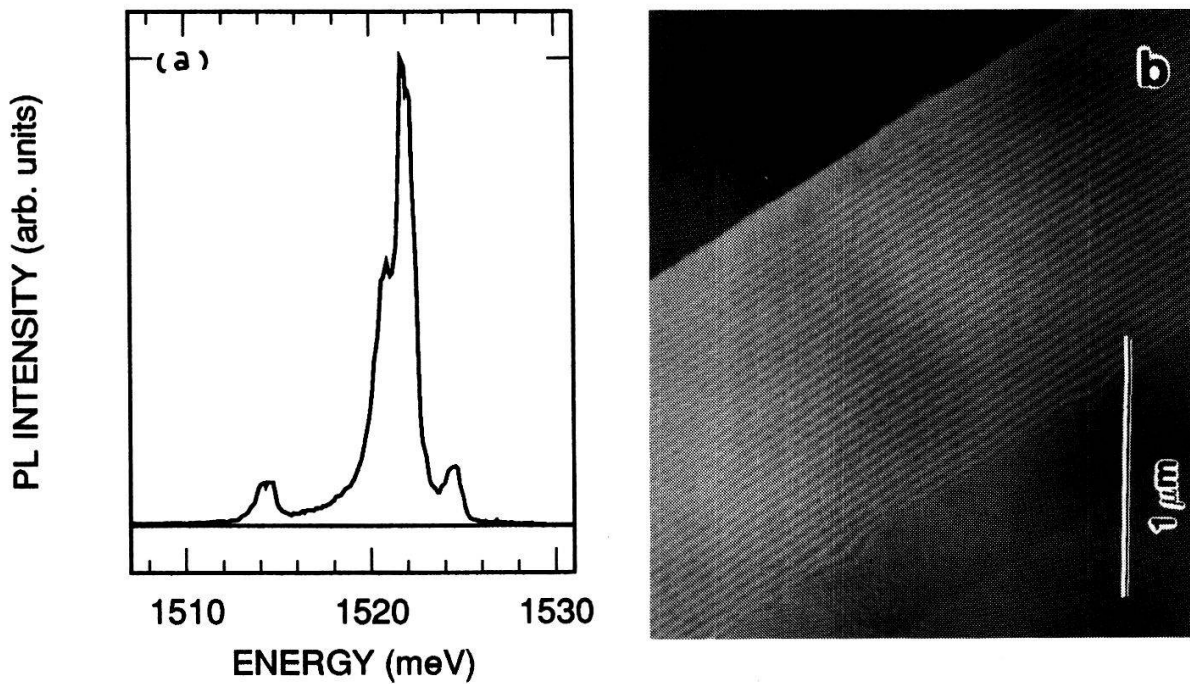


Fig. 1 Photoluminescence spectrum excited with $\lambda = 633$ nm at 4 K (part a) and Scanning Electron Microscopy photograph (part b) of the MQW sample.

heavy hole exciton X_{hh} (with a fine structure due to half monolayer interface fluctuations: at 1.5246 eV and 1.5221 eV) and the emission due to X_{hh} bound to a donor (1.5209 eV) [5]. At lower energies there is the luminescence of the $GaAs$ exciton bound to a donor. No luminescence from the $Al_{0.3}Ga_{0.7}As$ barriers or buffer layer was detected.

The Zn diffusions were performed by using the sealed ampoule technique in order to obtain reproducible conditions [6]. We used quartz ampoules outgassed and evacuated to about 10^{-6} Torr prior to sealing. The diffusion source was $ZnAs_2$ and the four temperature was $575^\circ C$. At this temperature the Zn diffusion coefficient in $GaAs$ is about $8.3 \cdot 10^{-13} cm^2 sec^{-1}$ and is even greater in $Al_xGa_{1-x}As$ [2]. We used different diffusion times.

3. Results and discussion

In Fig. 2 we show SEM photographs of our sample after 1 hour treatment (part a) and after 3 hours (part b). By assuming the diffusion constant quoted, we would expect a penetration depth for Zn (depth at which the Zn density is of the order of $10^{19} cm^{-3}$) of $\simeq 0.6 \mu m$ after 1 hour and of $\simeq 1 \mu m$ after 3 hours. It is known that layer disordering begin when the Zn concentration exceeds $10^{19} cm^{-3}$ [2]. Indeed, we observe in Fig. 2(a) that this is the case. After 1 hour 30% of the layers are destroyed and after 3 hours 90%.

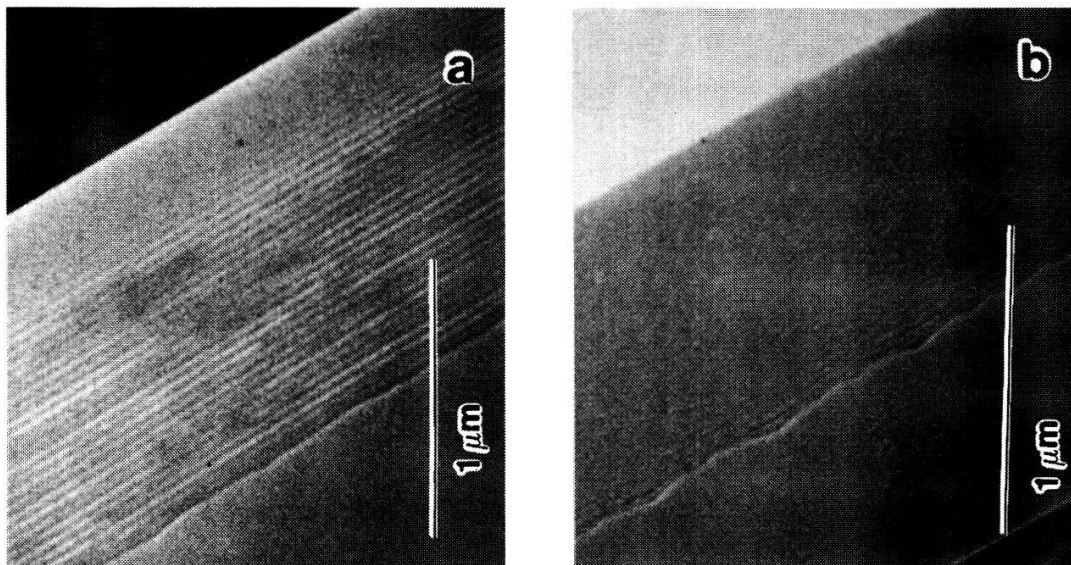


Fig. 2 Scanning Electron Microscopy photograph of the Zn diffused samples. Part (a) for one hour of diffusion and part (b) for three hours.

These results are confirmed by the PL measurements shown in Fig. 3. After one hours, see Fig. 3(b), the QW recombination dominates the spectrum. The strongest feature at 1.5185 eV is due to X_{hh} bound to the Zn acceptor [5], the two high energy emissions are due the X_{hh} and X_{lh} . Finally, the band at 1.5152 eV is due to the (e, A_{Zn}) recombination in which the Zn acceptor is in the barrier regions. By its spectral position we deduce an acceptor binding energy of about 15 meV which is in good agreement with theoretical calculations [5].

The spectrum of the sample diffused 2 hours is shown in Fig. 3(c). The high energy broad band is the (e, A_{Zn}) recombination in the $Al_yGa_{1-y}As$ disordered alloy with a mean Al concentration of $y \simeq 0.05$. We note that perfect $Al - Ga$ intermixing would results in $y = 0.07$. The low energy lines are due to, respectively, the $GaAs$ exciton bound to a donor recombination, defect exciton luminescence and (e, A_{Zn}) recombination with Zn in the well region (we obtain a binding energy of 30 meV). The defect exciton line, which dominates the spectrum, is caused by the high density of vacancy or point defects produced by Zn diffusion [1,2].

After three hours of Zn diffusion, almost all the layers are destroyed (see Fig. 2(b))

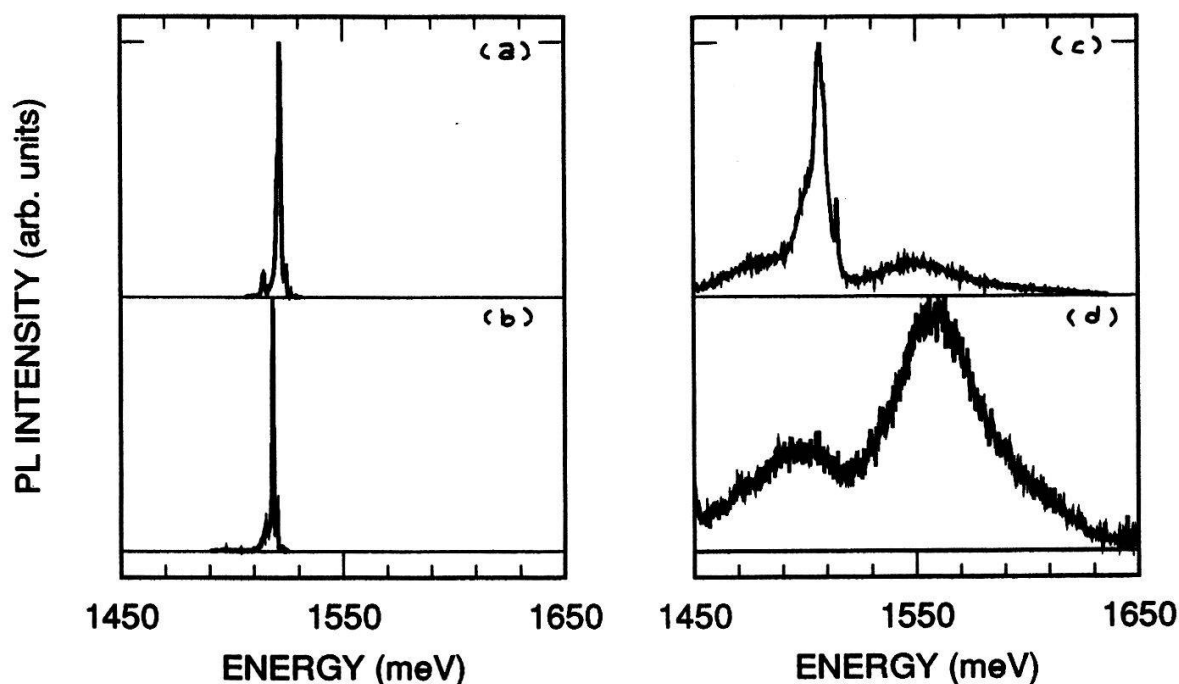


Fig. 3 Photoluminescence spectra at 4 K of the diffused samples. The different spectra correspond to different Zn diffusion times: (a) 0 hours, (b) 1 hour, (c) 2 hours, (d) 3 hours. The intensity scales are not related.

and in the PL spectrum (Fig. 3(d)) we observe two main features: a high energy broad band due to the (e, A_{Zn}) recombination in the disordered alloy (with an Al concentration of $y \simeq 0.06$) and a low energy band due to acceptor transitions in the GaAs buffer layers. We note also a strong reduction in the total PL integrated emission.

In conclusion we have shown that the details of the disordering process induced by Zn diffusion in QW layers can be studied by combining spectroscopical studies with SEM analysis. More work should be done in order to gain a better insight on the physics underlying impurity induced disordering.

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PROPERTIES OF HYDRODYNAMIC SYSTEMS WITH FLEXIBLE BOUNDARY
CONDITIONS

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Abstract: *In a circular channel we investigate experimentally the dynamics of a solid body which can move perpendicular to the axis of the channel. If the flow in the tube is slow and steady the stable stationary state of the system satisfies a variational principle. We show that at this state the Reynolds number reaches its maximum value. A generalisation of these results for bodies with deformable boundary conditions might have important applications in technical hydrodynamics.*

1. Introduction

It has been proved by Helmholtz and Korteweg /1/ that if the velocities at the boundary are given, the slow steady motion of an incompressible viscous liquid satisfies the condition of making the dissipation an absolute minimum. Feynman /2/ has shown, that the dissipation due to the Ohmic resistance reaches its minimum value at the steady state if the boundary conditions for the current are kept fixed. Recently it has been shown /3,4,5/ that the dissipation reaches a minimum at the stationary state too if the boundary conditions for the current vary essentially slower than the typical relaxation time of the distribution of the electric carriers. In this paper we investigate analogous hydrodynamic systems where the boundary conditions are not kept fixed but may change slowly compared with the typical time scales of the flow.

2. Experimental results

A solid body (Fig. 1) hangs on a thin wire ($\Phi = 0.1$ mm, length = 45 cm) in a vertical circular channel (Fig.2). The fluid is oil. With two valves the amount of oil Q

flowing through the channel is regulated. If the level of the oil in the channel stays on a constant value Q is nearly independent of the position of the solid body.

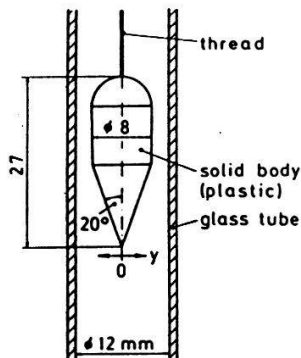


Fig. 1: Streamline shaped body (weight: 1.28 g) in a circular channel

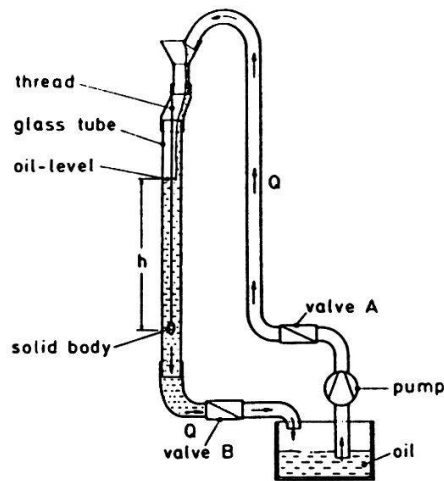


Fig. 2: Circular channel with a solid body

We investigate experimentally the stationary position y of the solid body for several values of Q . Fig. 3 indicates that the solid body approaches the boundary of the channel at low values of Q . At larger values of Q a position in the center of the channel seems to be stable.

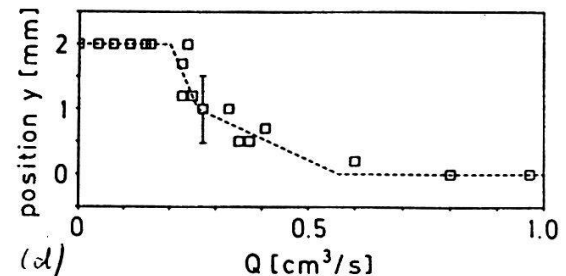
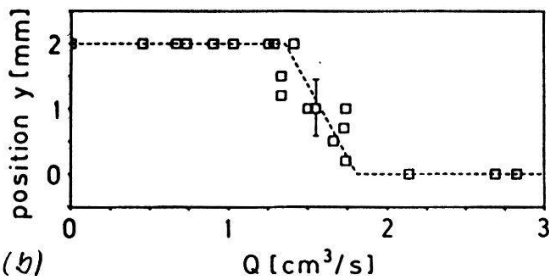
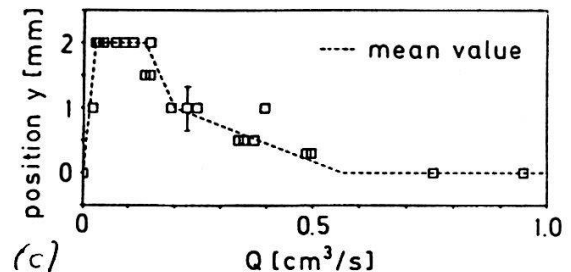
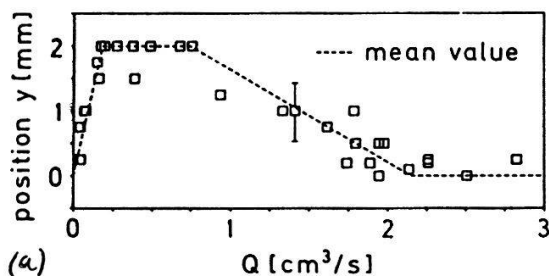


Fig. 3: The distance y of the center of the solid body from the center of the channel versus Q for two different liquids. Liquid A: viscosity $\eta = 0.045$ Pa s, density $\rho = 0.86$ g/cm³ (a,b); Liquid B: $\eta = 0.32$ Pa s, $\rho = 0.87$ g/cm³ (c,d). The stationary state for $Q = 0$ is at $y_0 = 0$ (a,c) and at $y_0 = 2$ mm (b,d).

3. Discussion

In order to explain the experimental results we use a simplified model. The outflow of an reservoir is divided into two channels by a plate which can move perpendicular to the axis of the channels (Fig. 4).

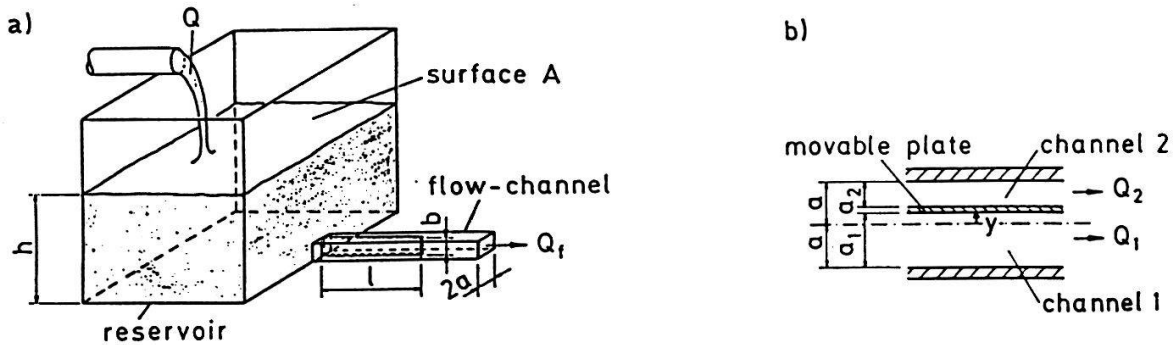


Fig. 4: A movable plate divides the outflow of a reservoir into two channels. The pressure at the end of the outflow is zero, Q is kept at a fixed value.

If the dynamics of the incompressible, viscous flow in the channels is estimated by the relations of a Poiseuille flow/6/ and the relaxation time of the motion of the fluid is essentially smaller than the typical time scale of the dynamics of the plate the potential energy can be estimated by:

$$V = c \cdot \frac{\eta^2 Q^2}{\rho} \cdot \frac{1}{(a^2 + 3y^2)^2} \quad (1)$$

where $c = 18 A l^2 / (g a^2 b^2)$ with the geometrical quantities A , l , a , b (see Fig. 4), gravitational constant g , viscosity η , density ρ and $|y| \leq a$.

In this case the motion of the fluid is slaved /7/ by the position of the plate. Therefore there is no explicit time dependence of V . If we assume, that V reaches a minimum at the stable stationary state we have $y = \pm a$ for stable stationary states, i.e. one channel is closed. In this case the dissipation

$$P = \frac{6 l}{a b} \cdot \eta Q^2 \cdot \frac{1}{(a^2 + 3y^2)} \quad (2)$$

reaches its minimum value too. In this simple system the dynamics of the plate models the dynamics of the solid body, the reservoir models the storage of the fluid in the real channel. The simple model seems to explain the stabilisation of the position at the boundary of the channel. Since the motion of the solid body is not exactly horizontal there is a small additional gravitational force acting into the direction of the position of the solid body for $Q = 0$. Therefore the position at the boundary becomes unstable for small Q if $|y_0| \neq a$. Up to now we have no explanation for the destabilisation of $|y| = a$ for large values of Q .

4. Conclusion

If gravitational forces can be neglected or if the solid body moves exactly horizontal, the solid body approaches a stable state at the boundary for small values of Q . At this state the Reynolds number reaches its maximum value and the dissipation its minimum value. The simple model indicates that a body with a deformable shape, e.g. a flexible cover with a medium of very high viscosity inside should approach a state with the same properties if the time scale of the deformation is essentially longer than the time scale of the fluid in the channel. An application of this effect might be the improvement of streamline shaped bodies.

We acknowledge H. Haken and O. Wohofsky for continuous support.

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RESONANT STIMULATION AND CONTROL OF KARMAN'S VORTEX STREET

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Abstract: We show that the periodic dynamics of a vortex street behind a circular cylinder can be modeled by a low dimensional system of ordinary differential equations with a few parameters, although the system has infinitely many degrees of freedom. The parameters depend on the hydrodynamic control parameters. We show experimentally that the dynamics is mainly on an inertial manifold. All degrees of freedom destinating away from the inertial manifold are slaved. Furthermore we show, that the system can be controlled by nonsinusoidal acoustic perturbations. The system remains on the inertial manifold if the perturbations are resonant.

1. Introduction

During the past several years there has been theoretical progress in hydrodynamics. Effinger and Großmann/1/ have calculated analytically the Kolmogorow spectrum for turbulent systems by a mean field theory. Furthermore, a huge variety of experiments shows, that there is an excellent agreement between theory and experiment for stationary and periodic systems/2,3/. In 1963 Lorenz/4/ pointed out that in the parameter region between periodic and turbulent state there might exist systems which can be modeled by strange attractors and low dimensional ordinary differential equations. Liapounov exponent and generalized dimensions indicate that there are low dimensional strange attractors in the Taylor-Couette system/5/, Benard system/6/, and the vortex shedding from a circular cylinder/7/. Recently a method has been presented for a reconstruction of nonlinear differential equations from experimental data/8/. The aim of this paper is to show that it is possible to reconstruct a differential equation from the dynamics of the flow of a vortex system behind a circular cylinder. Furthermore we show that the flow can be controlled/9/ in a very efficient way by using these differential equations.

2. Experimental results

The measurements have been done in the jet region of a wind tunnel which is similar to the wind tunnel of Eckelmann and Roesch/8/. The circular cylinder used has a diameter of 2 mm (steel, length=250mm) and is located 50 mm behind the outlet of the tunnel perpendicular to the jet. All velocity signals were obtained with a hot wire operated on a constant temperature anemometer. For nearly all signals, digitation was done on a sufficiently high frequency (10 kHz or more). The reconstruction of differential equations was done with the algorithm of Cremers et al. /10/. Smoothing and differentiating of the data were performed by a standard spline interpolation. The resulting flow vector field was approximated by a series of Legendre polynomials.

Fig. 1a shows a limit cycle drawn from the dynamics of the hot wire probe (Reynolds number $Re=70$). The position of the hot wire probe is in the center of the vortex street 6mm behind the center of the cylinder. 2000 data points which represent about 30 oscillations have been used to reconstruct an ordinary differential equation of the type

$$\ddot{v} = \sum_{i=0, j=0}^{3,3} a_{i,j} v^i \dot{v}^j \quad (1)$$

where $a_{i,j}$ are parameters. We estimated these parameters by a least square fit of the flow vector field resulting from the experimental data.

Fig 1.b shows the dynamics of the resulting differential equation. We found an excellent agreement between the geometry of the limit cycle of the measured data and the numerical simulation for various Re numbers ($0 < Re < 80$). Since most of the parameters vary strongly, may be due to experimental noise, we could not find a simple relation between the parameters of the differential equation and the Reynold number.

Further we investigated the response of the vortex system. We applied a sinusoidal

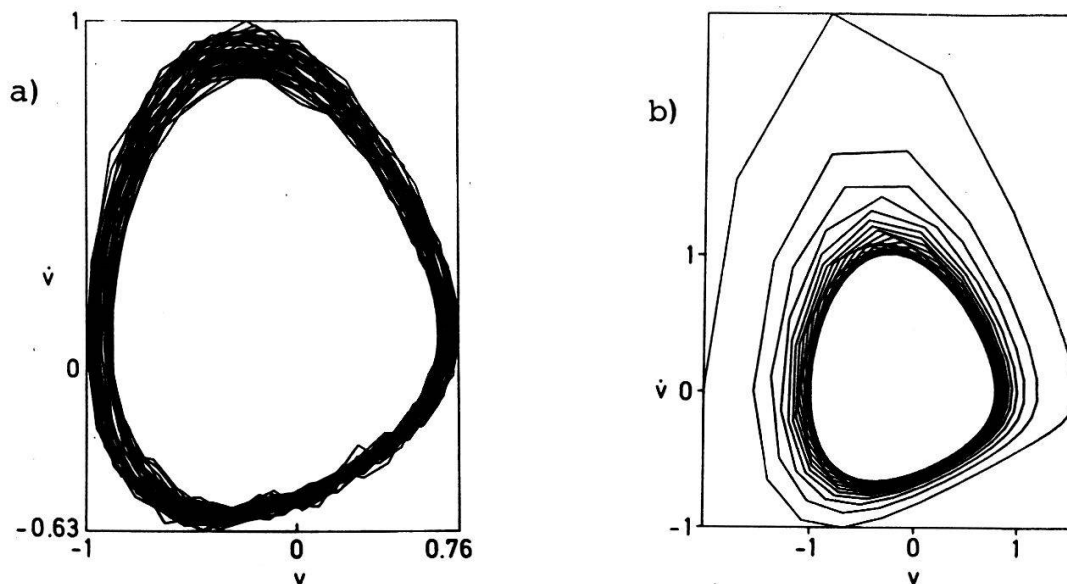


Fig.1 State space representation of the velocity signal v . v and $\dot{v}$ are normalized to their maximum value. (a) shows the experimental data and (b) a numerical simulation of the estimated differential equation.

and a square wave acoustic perturbation perpendicular to the flow by two loudspeakers. Fig.2a shows that the mode region of entrainment of a square wave response is essentially larger than the region of entrainment for sinusoidal perturbations. Fig. 2b shows the response of the vortex system to a very low frequency excitation. After the perturbation the dynamics is composed by a very low frequency motion and the usual quick oscillations. The low frequency motion is slowly damped out.

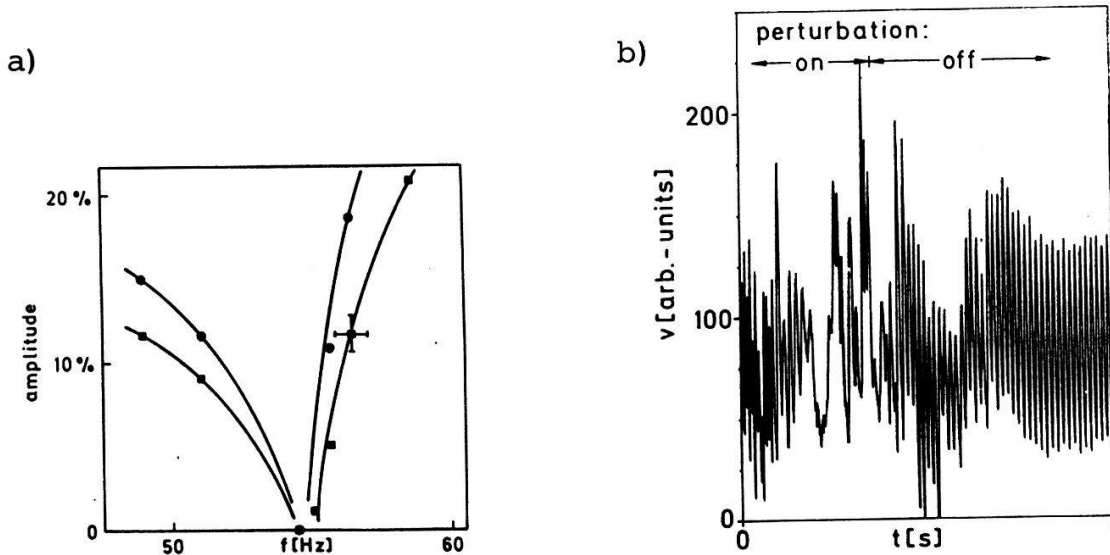


Fig.2a The boundaries of the region of entrainment for sinusoidal (●) and for square wave perturbations (■). The position of the hotwire is 6mm behind the cylinder in the center of the vortex street. The amplitude (distance between the extrema) of the acoustic perturbation is normalized to the amplitude of the variation of the velocity of the unperturbed system at this position. Fig.2b The response to a low frequency perturbation ($f = 0.1\text{Hz}$) versus time.

3. Discussion

The experimental results indicate that the dynamics of the velocity signal of the vortex street can be modeled by one dimensional oscillators with a nonlinearity up to third order since there is an excellent agreement between the limit cycle of the experiment and the limit cycle of the simulation. Fig. 1a indicates that the divergence of nearby trajectories is positive for $v > 0$ and negative else. Recently, it has been shown by nonlinear control theory that the region of entrainment of Van-der-Pol oscillators can be increased by a square wave perturbation/11/. The reason for the enlargement is that the divergence of nearby trajectories of the Van-der-Pol oscillator just depends on the amplitude $x(t)$ and is independent of the velocity $\dot{x}$. Since the differential equation of a Van-der-Pol oscillator and Eq.(1) are closely related and the divergence of both systems is nearly independent of the dotted variable this property might be the reason for the enlargement of the region of entrainment. From this discussion and from the successful

reconstruction of a differential equation from the experimental data we conclude that the dynamics of the velocity signal of the vortex street can be modeled by a low dimensional system of differential equations. Of course there are other excitations which are not included in such a simple model, as Fig. 2b indicates. The state space of hydrodynamic systems has an infinite number of degrees of freedom. The dynamics of the variables of the model is in a subspace, which is called inertial manifold. Fig. 2b indicates that it is possible to stimulate some degrees of freedom destinating away from the inertial manifold but it indicates further that these excitations are damped out after a while. We conclude that there is a large variety of degrees of freedom destinating away from the inertial manifold which are slaved/2/, which are not explicitly included in the model, but which can be excited by strong perturbations. However a general feature of the response of most real systems is, that the excitation is small if the perturbation is small. If the goal of the perturbation is to shift the basic frequency of the vortex street, the stimulation with square waves has two advantages: first, due to the enlargement of the region of entrainment it is possible to shift the frequency of the experimental system by a perturbation of small amplitude, and second, one can predict the response using a low dimensional system of differential equations since the excitations destinating away from the inertial manifold generally remain small. Generally nonlinear control theory /9/ provides us with the possibility to calculate perturbations which satisfy a certain condition or goal, but are of small amplitude. Usually these *resonant* perturbations are aperiodic but the amplitude of excitations destinating away from the subspace of the model remains small. May be perturbations of this type can be used to control chaotic flows.

We like to acknowledge H. Haken and O. Wohofsky for continuous support and W. Eberl for computer programs. Furthermore we acknowledge fruitful discussions with H. Eckelmann, E. Roesch, and R. Friedrich.

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+ part of Ph.D. thesis

RESONANT STIMULATION AND CONTROL OF NONLINEAR MECHANICAL PENDULUM BY POINCARÉ MAPS

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Abstract: A new method for resonant stimulation of nonlinear damped oscillators by nonlinear entrainment is presented. Appropriate driving forces are calculated with Poincaré maps. These maps can be extracted from experimental time series. We show experimentally, that the resonant driving forces are in phase with the velocity of the oscillator and cause a huge energy transfer. The corresponding driving forces are aperiodic and can be calculated without any feed back from the experiment.

1. Introduction

It has been shown numerically/1/ and experimentally/2/ that a nonlinear damped oscillator can be stimulated resonantly by nonlinear entrainment. For a large variety of nonlinear oscillators higher order Fourier amplitudes fall off rapidly/3/. The dynamics of these oscillators can be approximated by a smooth interpolation between the extrema of the exact dynamics. The extrema of the exact dynamics can be calculated with special Poincaré maps. The time between the extrema is the recurrence time of the Poincaré map. Since resonant driving forces are closely related to the dynamics of the unperturbed system they can be estimated from these Poincaré maps too/4/. The aim of this paper is to show experimentally that a resonant stimulation of nonlinear oscillators is possible, even if the resonant driving force is estimated from a Poincaré map.

2. The experimental setup

As a real physical nonlinear oscillator we used a damped wheel with a eccentric mass distribution/5,6/. The dynamics of the pendulum can be modelled by

$$\Theta \cdot \ddot{y} + \eta \cdot \dot{y} + c_1 \cdot y - c_2 \cdot \sin(y) = F(t) \quad (1)$$

where y is the angular displacement, $\Theta = 1.65 \cdot 10^{-3} \text{ kgm}^2$, $c_1 = 1.62 \cdot 10^{-2} \text{ kgm}^2 \text{ s}^{-2}$, $c_2 = 0.03563 \text{ kgm}^2 \text{ s}^{-2}$ and η the friction constant which can be varied in the range of $5 \cdot 10^{-5} \text{ kgm}^2 \text{ s}^{-1} < \eta < 6 \cdot 10^{-4} \text{ kgm}^2 \text{ s}^{-1}$. The time dependent driving force $F(t)$ is transmitted by a digital-to-force converter from a computer to the experimental pendulum.

3. Estimation of the driving force

3.1. Numerical estimation of the resonant driving forces

It has been shown / 1,2 / that driving forces $F(t)$ are resonant if $F(t) = (1 - \alpha) \cdot \eta \cdot \dot{x}$ where α is a real constant and where the dynamics of x is given by

$$\Theta \cdot \ddot{x} + \alpha \cdot \eta \cdot \dot{x} + c_1 \cdot x - c_2 \cdot \sin(x) = 0 \quad (2)$$

and where $x(0) \approx y(0)$. We integrate Eq. (2) numerically with a Runge-Kutta algorithm of 5.th - 6.th order and approximate the next-extrema map and the recurrence time between the extrema by a polynom of fifth order.

$$P_y: \quad \dot{a}_{n+1} = \sum_{i=0}^5 c_{n,i} \cdot (\dot{a}_n)^i \quad T_n: \quad T_n = \sum_{i=0}^5 c_{n,i} \cdot (\dot{a}_n)^i \quad (3)$$

where $\dot{a}_n$ is the n -th extrema, of the dynamics of $1.05 \cdot (1 - \alpha) \cdot \eta \cdot \dot{x}$ and T_n is the time between the $\dot{a}_n$ and $\dot{a}_{n+1}$. $F(t)$ results from a smooth spline interpolation between the data resulting from an iteration of Eq.(3). We took initial values for the iteration which are close to the stationary state of the unperturbed system.

3.2 Estimation of the resonant driving forces from the Poincaré map of the unperturbed system

For $\alpha = -1$ Eq. (2) results from Eq. (1) by a reflection of time. In this case the dynamics of $\dot{a}_n$ can be calculated from the dynamics of the extrema of $\dot{x}$ the unperturbed system by a reflection of time. $F(t)$ can be estimated by a smooth interpolation of the corresponding Poincaré map Eq. (3).

4. Experimental results

Fig. 1b shows the resonant stimulation of the pendulum ($\eta = 6 \cdot 10^{-4} \text{ kgm}^2 \text{ s}^{-1}$, $\alpha = -.17$) where the Poincaré map was calculated numerically. In Fig. 1a we depict the response of the experimental pendulum for $\eta = 3 \cdot 10^{-4} \text{ kgm}^2 \text{ s}^{-1}$ and $\alpha = -1$ where $F(t)$ was estimated from the dynamics of the unperturbed systems. Due to the strong amplitude frequency coupling [7] of the pendulum there is a sensitive dependence of the basic

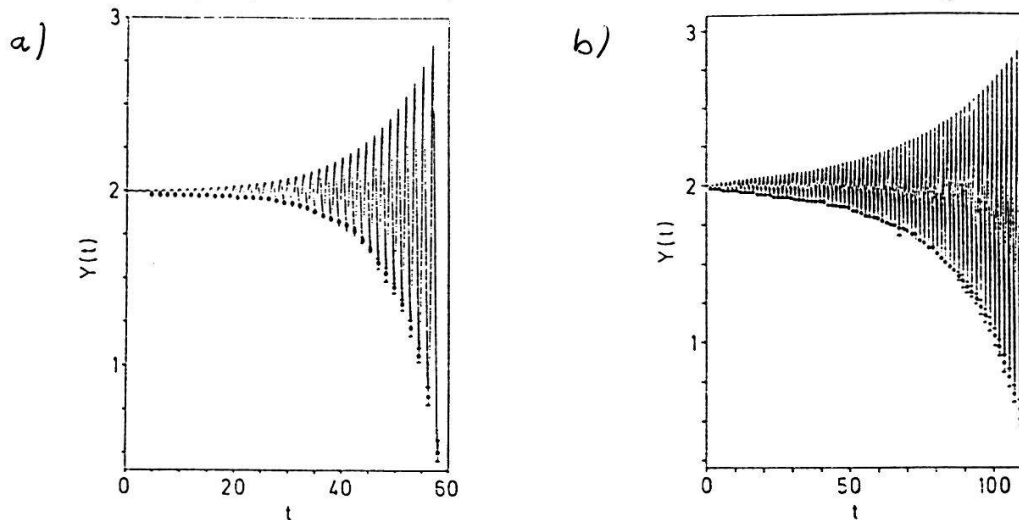


Fig. 1 The extrema of the amplitude y of the experimental pendulum versus t for $\alpha = -1$ (a) and $\alpha = -0.17$ (b). The continuous line represents the theoretical dynamics of y .

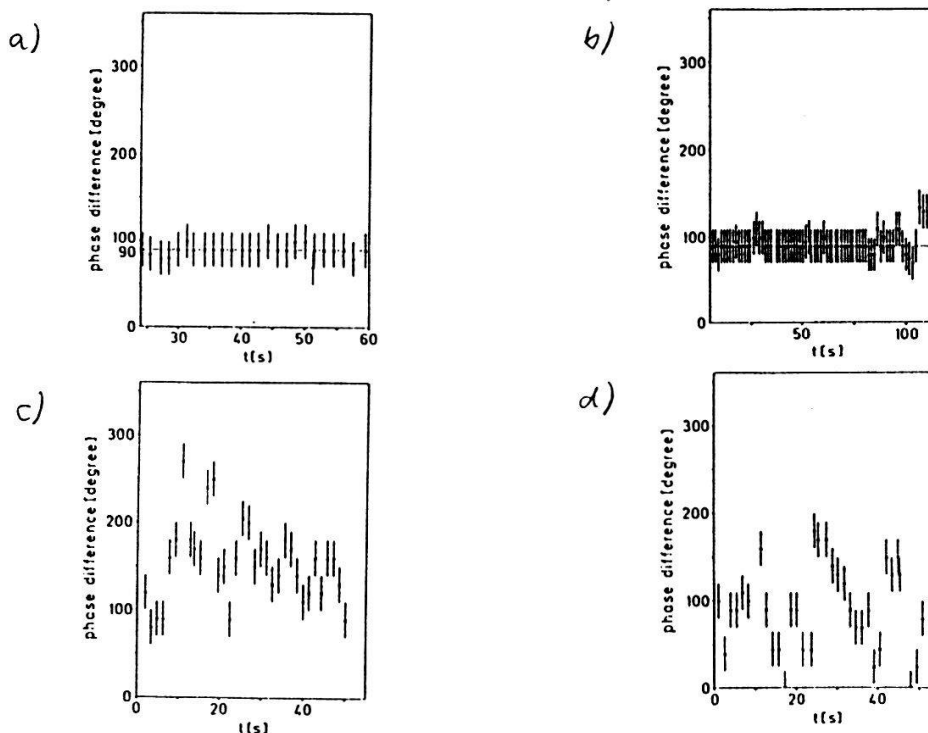


Fig.2 The difference in phase between F and y versus t . (a,b): Resonant stimulation by Poincaré-Map, (a): $\alpha = -1$, $\eta = 3 \cdot 10^{-4}$. (b): $\alpha = -.17$, $\eta = 6 \cdot 10^{-4}$; (c,d): Sinusoidal stimulation with $F = 4 \cdot \sin(\omega_0 \cdot t)$, ω_0 : eigen frequency in the linear region, (c): $\eta = 3 \cdot 10^{-4}$, (d): $\eta = 6 \cdot 10^{-4}$.

frequency of the oscillator from the amplitude of the oscillation. Fig. 2 illustrates that the phase relation between the driving force and y remains 90 degree, despite of the large shift in frequency. The phaseshift of 90 degree between y and F indicates that the reaction power is zero and that the driving force is resonant/1/. If the driving force is sinusoidal this resonance condition is not satisfied (Fig. 2c,d).

5. Conclusions

We have shown that nonlinear oscillators can be stimulated resonantly by driving forces which are estimated from Poincaré maps. These Poincaré maps can be estimated analytically/8/, numerically or directly from the unperturbed system. Therefore the stimulation can be done without any idea on the differential equation of the system. No direct feed back from experimental system is necessary during the stimulation. If the Poincaré map has been estimated, the whole time dependence of the driving forces can be calculated before the stimulation starts.

We like to thank H.Haken and O.Wohofsky for continuous support.

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Formation of Selfsimilar Dendritic Patterns with Extremal Properties

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Abstract

Under the influence of an electric current I small metallic balls form a stable, stationary dendritic pattern exhibiting extremal properties. The corresponding quantity as well as the fractal geometry are experimentally studied as a function of time and the control parameters of the system. The results are compared to those obtained for transient dendritic structures, e.g. electro-deposits.

1 Introduction

Dendrites form ramified, simply connected patterns that are selfsimilar within a certain range of length scales. Obeying a merely deterministic law, modulated by stochasticity, the growth of transient dendritic structures is a manifestation of chaos. It can be shown that under certain conditions the slaving principle, first introduced by *Haken*, applies leading to a stationary dendritic structure, characterized by an extremal property /1,2/. Here the temporal development of those structures has been studied experimentally.

2 Brief Theoretical Review

Under the influence of an electric field, charged particles agglomerate thus forming a ramified, open structure. Since the basic equations for the agglomeration process of the charged particles are closely related to diffusion processes, the structure formation can be described by a DLA model /3/, if the particles belonging to the cluster cannot move anymore.

An experimental example for such a process is electro-deposition /4/. For a quasi two-dimensional dendritic copper electro-deposit grown by electrolysis, the reservoir of Cu^{++} ions (the electrolyte $CuSO_4$ and the copper anode) is practically infinite and it is possible

to define a dynamical fractal dimension D_{dyn} by $\langle r \rangle \sim t^{1/D_{dyn}}$, where $\langle r \rangle$ is the average extension of the dendritic cluster formed, and t is the time elapsed since the start of electrolysis. The geometrical fractal dimension D remains more or less constant during the whole of this process, both under the constraint that growth parameters (such as ion current I or electrolyte concentration c_{CuSO_4}) are not varied. From this it must be concluded that the structure, once formed, keeps its characteristics, i.e. no detectable restructurizations take place [5].

Things are completely different, if the agglomerate can move around and the particles' movement is slowed down by a large and isotropic frictional force. We assume that the dynamics of the agglomerating particles can be modeled by an equation of motion of type

$$-\gamma \dot{\vec{q}}_i - \vec{\nabla}_{\vec{q}_i} V = 0 \quad (1)$$

Here γ is a large friction constant, $\vec{q}_i$ is the position of the i^{th} particle, $V = V(\vec{x}, \vec{q}_i(t); t)$ is the potential energy of the system and $\vec{x}$ a point in space. As the damping constant γ is very large, the relaxation time of the mechanical degrees of freedom exceeds that of the electrical ones, and the latter are slaved by the first [6]. Thus two different time scales may be separated, and the potential energy V loses its explicit time dependence and becomes a *Lyapunov* function of the system. That is the particles attain a stable stationary state, characterized by minimal potential energy,

$$\dot{\vec{q}}_i = 0 \quad \Rightarrow \quad -\vec{\nabla}_{\vec{q}_i} V = 0 \quad \Rightarrow \quad V \text{ extremal.} \quad (2)$$

3 Experiments and Results

The experimental set-up described in [2] has been used to study the temporal development of such a dendritic structure until the stationary state is attained:

Under the influence of a constant electric current, I , N mesoscopic electrically conducting balls ($\varnothing = 2 \text{ mm}$, $N = 600$) – initially statistically distributed in a round acrylic dish ($\varnothing = 114 \text{ mm}$), filled with the viscous and poorly conducting castor oil up to a height of about 3 mm , – cooperatively form a dendritic structure. The current I is produced between a metallic tip, at height $h = 40 \text{ mm}$ in the air above the center of the dish, set to potential U , and a grounded ring electrode at the inner edge of the dish. The agglomerate of all directly or indirectly grounded balls (referred to as grounded balls) may be characterized by its geometrical fractal dimension D . D is determined by a box-counting-algorithm. Two other characteristic properties are the number of open ends M and the resistance R when collecting the charges sprayed upon the oil surface and conducted to the ground (determined by a numerical solution of the *Poisson* equation). This resistance is proportional to the electric potential energy V [2], $R \sim V$. Thus, from equation (2), R will also be minimal for the stationary state. The temporal development of these three quantities has been monitored for four different applied voltages ($U = 12.5, 15.0, 17.5, 20.0 \text{ kV}$), where U has been regulated so as to keep I constant.

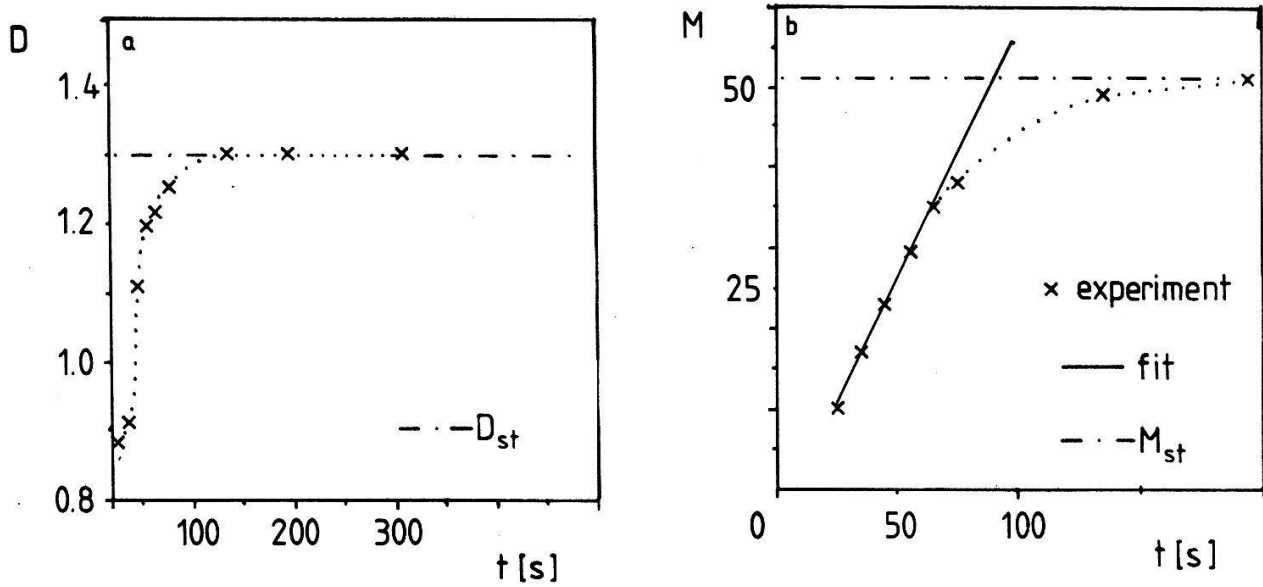


Figure 1: Temporal development of fractal dimension D (a) and number of open ends M (b) for an applied voltage $U = 12.5 \text{ kV}$, the stationary state being characterized by D_{st} and M_{st}

When starting the experiment, the balls begin to attach to the ground and to grounded balls. They stick preferentially to the largest branch formed, i.e. where the sticking probability P_{stick} is largest. Therefore there is usually one grounded system, much larger than all others. When more or less all particles are part of the cluster, some balls still modify their positions slightly in order to minimize their potential energy V . The pattern attains the stationary state and is asymptotically characterized by the constant values D_{st} , M_{st} and R_{st} , which depend only on the charge current I traversing the dendrites (hence on U and the height of the tip h). In figure 1 this temporal development of the fractal dimension D (a) and the number of tips M (b) is plotted for an applied voltage $U = 12.5 \text{ kV}$, showing clearly the two different regimes. The first regime is determined principally by a DLA like process, because there are almost no restructurizations to be observed. Whilst the second regime, where only slight modifications of the structure take place, leads to the values D_{st} and M_{st} asymptotically, which are independent of the initial conditions A ,

$$D(A, t; U) \rightarrow D_{st}(U) \quad ; \quad M(A, t; U) \rightarrow M_{st}(U) . \quad (3)$$

Because of equation (2) and the proportionality, $R \sim V$, the resistance R_{st} is the quantity best able to describe the stationary pattern, characterized by minimal potential energy V . Its formation process is sketched in figure 2(a) for $U = 15.0 \text{ kV}$. Here the stationary state, $R(A, t; U) \rightarrow R_{st}(U)$, is developed earlier than in figure 1 because of the higher voltage applied. In figure 2(b) the time t_1 , when the fractal dimension $D = 1$ is reached, is sketched as a function of U . For $U < 12 \text{ kV}$ no growth process is initiated, for $U > 25 \text{ kV}$ the ionization of the air is too high to carry through the experiment without any supplementary precautions.

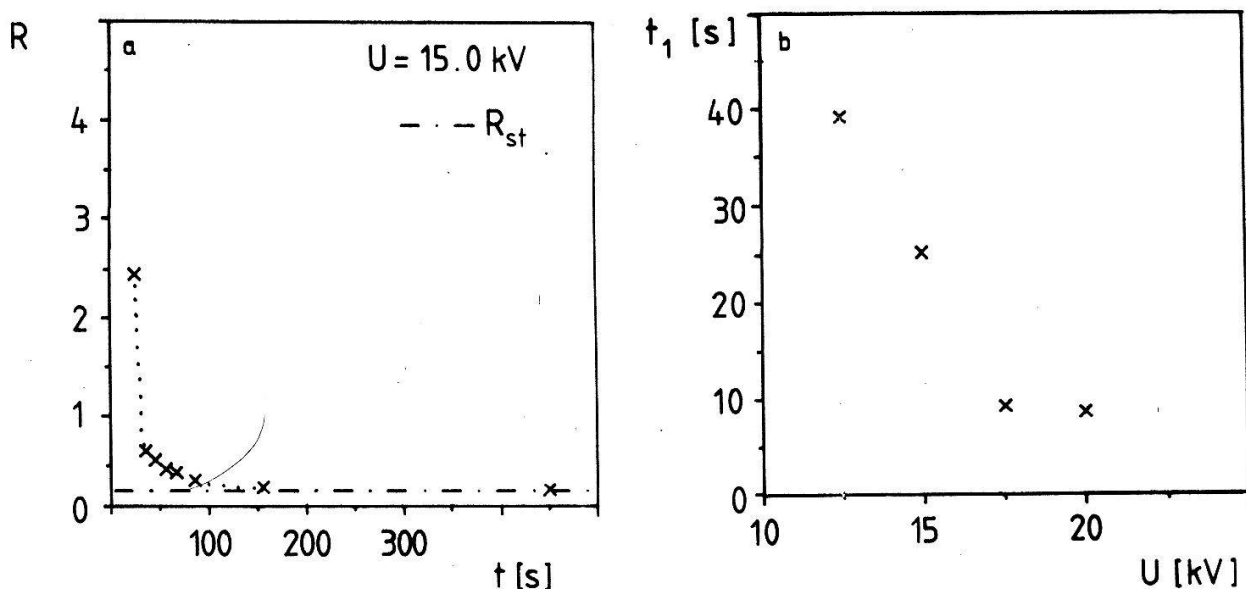


Figure 2: a) Temporal development of the resistance R ; b) time t_1 , when the fractal dimension $D = 1$ is reached, as a function of the applied voltage U

4 Conclusion

When damping is high, dendritic structures may asymptotically reach a stationary state, characterized by an extremal property. In this case two different regimes may be distinguished. The first regime is essentially determined by a mere aggregation process, whilst the second regime consists only in slight modifications of the structure.

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Acknowledgement

The authors like to express their thanks to Professor Dr. H.Haken for his helpful hints, to Dr. O.Wohofsky for his interest in their work, to W.Eberl for his supply in computational problems and to P.Hildebrand for his help, when evaluating the experimental results.

Digital temperature controller for low temperature experiments

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Abstract: our temperature controller measures simultaneously 4 Ge or carbon glass resistors with continuous cancellation of thermal EMF, very low power dissipation and a precision of 10^{-4} between 100Ω and $50k\Omega$, which correspond to $\approx 1\text{mK}$ below 10K and even better at lower temperature. The voltages across the sensors are amplified and converted to frequencies which are measured 10 to 50 times/s, a rate well suited to systems of low heat capacity. The regulation is performed numerically and independently for each sensor through heaters powered by digital to analog converters. A global calibration of the system can be performed even during an experiment.

Introduction

Temperature measurement and control is not a simple task if a precision in the mK range and fast convergence to a set value are required. The difficulty comes from the many requirements, difficult to fulfill at the same time. For example the need of high precision under very low power dissipation to avoid self-heating of the sensor imply low current and voltage and very low noise, while low specific heat encountered at low temperature may require up to 50 measurements/s.

Germanium or carbon glass resistors are widely used as temperature sensor and their stability is such that they can be used as secondary standard at low temperature, with a reproducibility better than 1 mK. Their resistance is a complicated function of temperature that can be –after calibration– fitted by a polynomial equation based on Chebychev polynomials [1]. So conversion from resistance to temperature and the converse are possible.

Between 20K and 1K, the sensitivity dR/dT of these devices changes by orders of magnitude. It is also the case for specific heat and thermal conductivity of materials, so an analog temperature controller with constant proportional, integral and differential (PID) parameters may become unstable below a certain temperature.

Electronic temperature controllers have been reported in the literature [2,3] or are commercially available [4,5,6]. Some of them feature a digital regulation by turning on and off a heater which may cause noise and oscillations of the temperature; others feature an analog regulation with the possibility to adjust the set point and the gain or reset the integral by software. Only one [2] feature a digital regulation with an analog output to a heater, but is not suited to low temperature experiments.

We present a microcomputer-based temperature controller that gives the flexibility to limit the power dissipation in the sensor to 10^{-7} watt at 4 K and to lower values (10^{-10} watt) below 1 K to avoid self-heating, while maintaining the overall accuracy to 10^{-4} by cancelling thermal EMF and amplifier drift. It allows the conversion of resistance to temperature and vice versa. The regulation is done by calculating the amount of heat sent by a Digital to Analog

Converter (DAC) to a heater. The micro-computer gives the flexibility to build a complex regulation by software.

Measurement of resistance

The simplest way to measure a resistance consists in injecting a known current through it, amplifying the voltage developed across and measuring it.

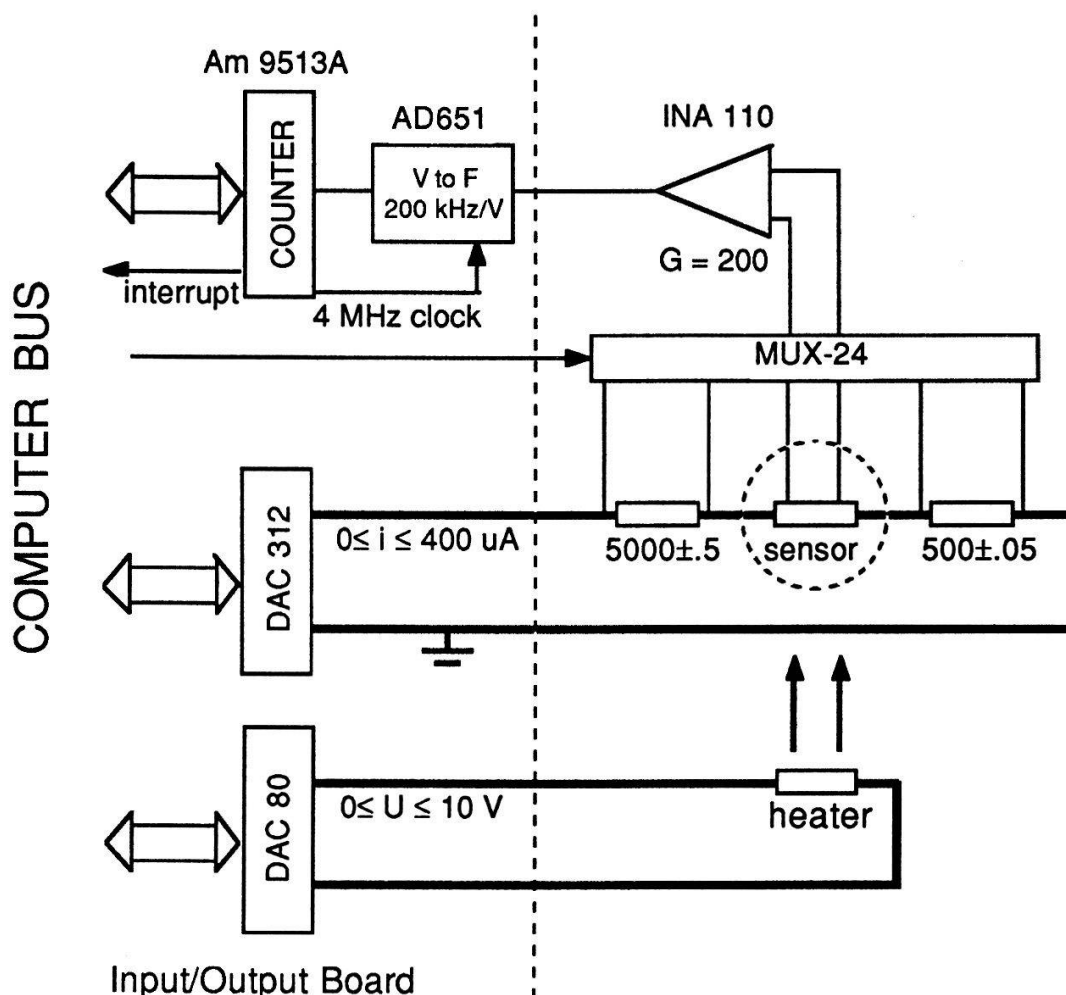


Figure 1: block scheme for one thermometer loop. The I/O board contains four current sources (DAC312), four VtoF and four DAC80 used for the heater. One timing controller Am9513A is used for the four channels. The precision resistors, MUX-24 and instrumentation amplifiers INA110 are in a box near the top of the cryostat.

After many trials with operational amplifiers we found that the best and simplest current source is a DAC with true current output, ie with large output impedance and voltage compliance like PMI DAC08 or DAC312. The stability of 10 ppm/K is well suited and there is no problem of oscillations encountered very often with operational amplifier design. The absolute precision is about 10^{-3} with a full scale current, decreasing to 10% with only the last

significant bit on. An individual calibration of each of the 8 or 12 current sources of the DAC allows to reach the required precision. The current can be switched off to measure offsets.

We use an intermediate box, between the cryostat and the computer to amplify low level signals and avoid pick-up noise from computer boards. This box contains instrumentations amplifiers Analog Devices AD624 or Burr-Brown INA110 characterized by low bias current, low noise, low gain drift and, fast settling time. Two high precision (10^{-4}) resistors of 500Ω and $5K\Omega$ are serially connected in the current path and a multiplexor MUX 24 of PMI allows to switch either the thermometer or one of these resistors at the input of the INA110 (see figure 1). It is possible to add RC filters on the four lines of the sensor, at the top of the dewar, to avoid RF picked-up voltages to heat the sensor. This proved to be useful below 0.5 K.

The need of very low noise ($\leq 1\mu V$) and medium speed (10 to 50 reading/s) required us to use voltage to frequency (VtoF) conversion and to count the number of pulses in a period Δt which is a multiple of line period (20ms in Europe) in order to reject the noise at line frequency. A system timing controller Am9513A provides five independent 16 bits counters and allows to count simultaneously 4 different signals gated by the 5th counter which produces an interrupt to the processor after Δt when a new measurement is ready. Normally there is no relation between input frequencies and gate frequency so that metastable states (when the storage device is clocked in close temporal proximity to changes on the data input) may occur and the value read by the counter is wrong. The probability of such event is proportional to the input frequency ($\sim 1\text{MHz}$) times the gate frequency ($\sim 50\text{Hz}$) times the metastable state ($\sim 75\text{ pS}$ for Am9513A). So under these conditions the average time between two wrong readings is about 270s. To avoid these troubles we used a synchronous VtoF (AD651) with the same clock as the counter.

Rather than calibrate the current i , the gain of the instrumentation amplifier and the VtoF conversion rate, we just switch the multiplexer to a calibration resistor and obtain an overall calibration in counts/ohm for a given current and Δt . Calibration can be done during measurements.

The hardware was first implemented on Texas TM990 microcomputer. The real time operating system PDOS allows to create tasks and to suspend them until an hardware event is coming (interrupt). So different tasks can be executed concurrently, the highest priority being the first. The task to measure or control a temperature can be a part of a more complex data acquisition system [7]. The same operating system exists now on VME bus. So we did develop recently a board for that bus. The programs are now written in Pascal.

A measurement cycle starts with few readings with zero current to estimate the average X_0 with a good precision. The smallest current (100nA) is then switched on and X_0 is subtracted from each subsequent measurement X_m to obtain the net value $X_r = X_m - X_0$. The program can calculate the resistance R corresponding to X_r and the temperature by Chebychev polynomials. Depending on the temperature, the program can select a current as high as possible to have a good resolution but low enough to avoid overloading of the counter and self-heating of the sensor. The measurements with zero current are repeated every 10 s to cancel drifts and thermal EMF.

Control of temperature

To set a temperature T_c , the program calculates the corresponding resistance R , the appropriate current and X_c , the value to be read by the counter when T is equal to T_c . X_c is a 16 bits integer and all the regulation is done with 32 bits integer arithmetic to minimize the computing time. From the net reading X_{ri} , the program calculates the error Δ_i and it's variation $d\Delta_i$ between two successive measurements.

$$\Delta_i = X_{ri} - X_c$$

$$d\Delta_i = \Delta_i - \Delta_{i-1}$$

As mentioned above, heat capacity and thermal conductivity have orders of magnitude variations between 0.1 K and 10 K. If the cooling power is due to a constant molar flow rate of for example ^4He through an impedance, the relation between the heating power H is nearly independent of T up to a value where T starts to rise sharply. Until now we have used the following algorithm to calculate H :

$$H = \Delta_i \cdot \text{cstP} + \sum_{\text{sat}} (\Delta_i \cdot \text{cstI} + d\Delta_i \cdot \text{cstD} \cdot |\Delta_i|) \quad (1)$$

The first term ($\Delta_i \cdot \text{cstP}$) is proportional to the error. The subscript sat means that the sum is limited between zero and a maximum value. The second term correspond to the integral of the error and the third term is used to minimize the overshoot by dumping the integral. X_r converge to X_c if $d\Delta_i \cdot \Delta_i < 0$. In that case, if after N measurements $X_{r(i+N)}$ will not cross the set value X_c (or $N \cdot |d\Delta_i| < |\Delta_i|$) the program set $\text{cstD} = 0$. If X_r will cross the set value X_c before N measurements ($N \cdot |d\Delta_i| \geq |\Delta_i|$) or if the absolute value of the error increases ($d\Delta_i \cdot \Delta_i > 0$) the third term becomes effective.

This algorithm is empirical but gives very fast convergence to a few mK in about 10 s. It is possible to find constants (cstP , cstI , cstD , N) valid for a large temperature range but, to optimize the convergence (smallest time, no overshoot), we have to adapt these constants to the temperature. We are looking for algorithms to find them automatically but, as is, the system regulates well. The measurement and control of four temperatures 50 times per second use less than 7% of the CPU time (99105 CPU @ 6 MHz or 68000 CPU @ 8 MHz).

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NUMERICAL CALCULATION OF ELECTRICAL BREAKDOWN IN OXYGEN IN A DIELECTRIC-BARRIER DISCHARGE

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Abstract: We briefly state and formulate the numerical problem of calculating the breakdown currents and fields generated by applying high fields to plane-parallel gaps in which one of the electrode is covered by a dielectric. Such a discharge consists of a number of randomly distributed microdischarges. The aim is to calculate the temporal behaviour of one such microdischarge.

1. Introduction

We consider a plane-parallel arrangement of two electrodes (Fig. 1). One of the electrodes (here the anode) is covered by a dielectric of thickness g . The gap between the cathode and the dielectric is filled with oxygen of approximately atmospheric pressure. We apply a constant voltage between the electrodes in such a manner that the electric field strength in the gap exceeds the Paschen-field. The Paschen-field is the minimum field necessary for a gap of this width and pressure to break down, i.e. to form self-sustaining electron avalanches. In our case the avalanches that develop transport charge to the dielectric surface. This surface charge induces a field which is directed opposite the applied field. Thus, after a certain charge has been deposited on the dielectric, the effective field becomes lower than the Paschen-field and the discharge extinguishes i.e. the electron current decreases to zero. The current pulse thus generated has a duration of only a few nanoseconds. In what follows we will give a brief description of the numerical approach used to solve the relevant equations. A similar problem was formulated in Ref. [1].

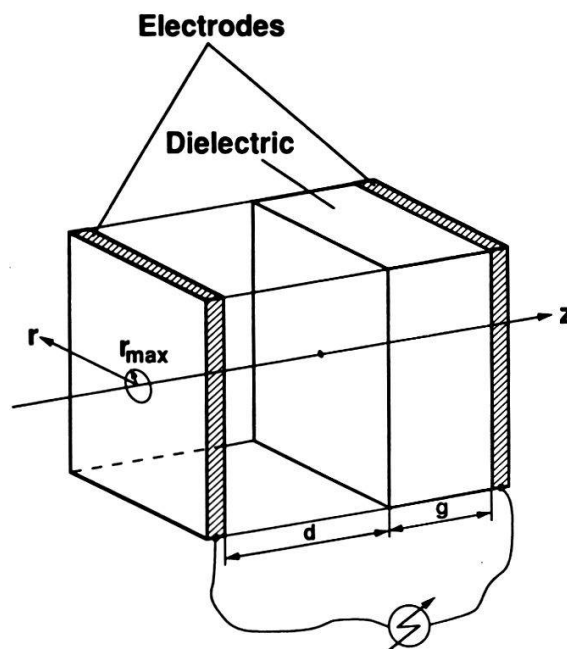


Fig. 1: Definition of the coordinate system and the geometrical parameters used in the calculations.

2. The Equations

To initiate a discharge we release a certain number of electrons n_{e0} from the cathode. These electrons ionize the oxygen molecules and thus start an electron avalanche.

The equations governing the behavior of charged particles in an electric field are the equation of continuity for the electrons (n_e) and the ions (n^+ , n^-) and the Poisson equation for the electric field.

By making the following assumptions: a) no diffusion, b) no ionic drift, c) constant electron mobility, i.e. $\mu \neq \mu(E/n)$ we get a simplified set of equations:

$$\frac{\partial n_e}{\partial t} + \text{div} (\mu \vec{E} n_e) = \bar{\alpha} \mu \vec{E} n_e \quad (1)$$

$$\frac{\partial N}{\partial t} = \bar{\alpha} \mu E n_e \quad (2)$$

$$\text{div} \vec{E} = \frac{e}{\epsilon_0} (N - n_e) \quad (3)$$

where $\bar{\alpha} = \alpha - \eta$ is the effective ionization coefficient and $N = n^+ - n^-$.

3. The Electron Density

It is easier to discuss the numerical approach in case of the one-dimensional problem. We will solve the equation of continuity by the method of characteristics. The above partial differential equation becomes an ordinary differential equation if we let the coordinate system drift with the electrons, i.e. by choosing $dz/dt = \mu E$. By considering Eq. (4) and that the ionic space charge $N=N(z)$ changes along the characteristic one gets the following differential equation

$$\frac{dn_e}{dt} = a n_e + (b + ct) n_e^2 \quad (4)$$

with the solution

$$n_e(t) = \frac{n_e^0 \exp(at)}{1 - \frac{n_e^0}{a} \left[\left(b + ct - \frac{c}{a} \right) \exp(at) - b + \frac{c}{a} \right]} \quad (5)$$

where $a = \bar{\alpha} \mu E - \mu \frac{e}{\epsilon_0} N$, $b = \mu \frac{e}{\epsilon_0}$ and $c = -b \bar{\alpha} \mu E$.

The spatial coordinate net, $z_i = i\Delta z$, is fixed. The time interval Δt is chosen such that the condition $\Delta t \mu E < \Delta z$ is fulfilled all over the spatial dimension. We use Eq. (8) for each integration step by taking $t = \Delta t$. We determine n_e^0 at the coordinate $z_i - \Delta t \mu E$ from a linear interpolation between the values at (z_{i-1}, z_i) in case of $\mu E > 0$ and (z_i, z_{i+1}) for $\mu E < 0$.

4. The Boundary Condition at the Dielectric

The boundary condition is

$$\epsilon_1 E_z(d_-) = \epsilon_2 E_z(d_+) + q \quad (6)$$

where q is the surface charge density on the dielectric and $z = d_-$ and $z = d_+$ resp. are the

planes immediately to the left or right resp. of the dielectric surface. In the one-dimensional case we have $E_z = \text{constant}$ inside the dielectric. Therefore we only have to solve the Poisson equation in the gap with homogenous boundary condition. The potential ϕ_0 at the dielectric surface on the gap side, i.e. for $z = d_-$ is

$$\phi_0 = \frac{U_0 \epsilon_r - g \left(\frac{q}{\epsilon_1} + \frac{\partial \phi}{\partial z} \Big|_{d_-} \right)}{\epsilon_r + g/d} \quad (7)$$

where U_0 it is the total potential between the electrodes and $\epsilon_r = \epsilon_2/\epsilon_1$. The electric field at the dielectric is

$$E(d_-) = - \left(\frac{\phi_0}{d} + \frac{\partial \phi}{\partial z} \Big|_{d_-} \right) \quad (8)$$

In the two-dimensional case we use cylinder coordinates r and z . The total charge on the dielectric is here $Q(t) = 2\pi \int_0^{R_{\max}} q(r, t) r dr$ where the charge density $q(r)$ is given by

$$\frac{dq(r)}{dt} = e\mu E(r, d, t) n_e(r, d, t) \quad (9)$$

and $R_{\max}$ is the outer radial boundary of the volume under consideration.

We determine the potential distribution by assuming a potential ϕ_0 at the boundary $z = d_-$ and using a fast Poisson solver (HSTCYL [2]) in the gap and in the dielectric resp. These solutions together with the boundary condition (9) allow us to determine the potential $\phi(d, r) = \phi_0(d, r) + \psi(r)$ in such a way that Eq. (9) is fulfilled, viz.

$$(\epsilon_1 J_1 - \epsilon_2 J_2) \psi = \epsilon_1 \frac{\partial \phi}{\partial z} \Big|_{z=d_-} - \epsilon_2 \frac{\partial \phi}{\partial z} \Big|_{z=d_+} + q \quad (10)$$

where J_1 and J_2 are the Jacobi matrices. For one integration step 3 HSTCYL calls are necessary.

5. The Boundary Condition at the Cathode

We assume that the electrons at the cathode are given by two terms, viz.

$$n_{e0}(0, r, t) = n_{e01}(r, t) + n_{e02}(r, t) \quad (11)$$

The first term n_{e01} is Gaussian in the radial direction. The other term, n_{e02} , constitutes the emission of electrons released from the cathode by photons generated in the gap. We assume n_{e02} is of the form $n_{e02}(r, t) = n_{02} \exp(-\beta r)$ where the amplitude n_{02} is given by [3]

$$n_{02}(t) = \frac{\gamma_{ph}}{v_d(0, t)} \int_0^d \alpha v_d n_e dz \quad (12)$$

The integral, which basically should be taken over the whole volume of the discharge, is approximated by the maximum integral in the z -direction we have also always taken the drift velocity at the cathode, $v_d(0, t)$, equal to the maximum value. The constant β was chosen between 1 cm^{-1} and 100 cm^{-1} .

6. Results

In Fig. 2 we show some results for the electron density $n_e(z, r, t)$. The data for oxygen have been taken from [4].

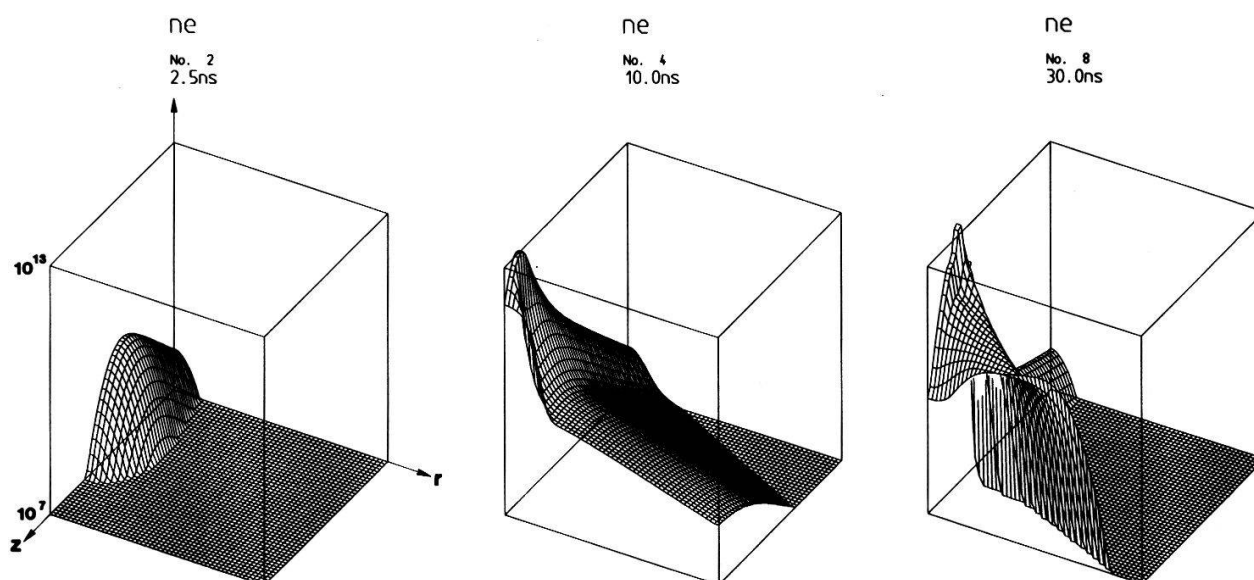


Fig. 2: The distribution of the electron density as a function of z, r, t for $d = 1 \text{ mm}$, $g = 0.8 \text{ mm}$, $\epsilon_r = 3$, $\beta = 100 \text{ cm}^{-1}$, $R_{\text{max}} = 0.4 \text{ mm}$ and an applied field of 155 Td .

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NUCLEATION IN SUPERCOOLED METALS WITH HIGH MELTING POINT

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Abstract: We have measured the cooling rate of supercooled droplets of metals with high melting point and the measurements of the limit temperature to the supercooling are lower than that predicted from the "classical" theory of nucleation. These measured cooling rates also present a temperature jumping just on the liquid-solid transition "point" and this behaviour appears to represent the nucleation process as an adiabatic one.

1. Introduction.

A problem of particular interest from the standpoint of the nucleation theory is that of determining the conditions under which the metastable state is thermally stable with respect to a transition to a stable state. To the liquid-solid transitions, the interest stems primarily from the thermal instability of the supercooled liquid and how this instability determines the maximum attainable depth of penetration into the metastable state, and fixing then the so-called limit temperature T_L to the supercooling.

In a recent series of experiments(1) we have measured the supercooling of metal droplets with high melting point using a contamination-free technique involving radiating freely falling liquid spheres. In the present study we have improved our observations of the supercooling and have extended a theoretical analysis of the results using both "classical" and adiabatic nucleation theories.

2. Experimental Procedure.

Each of the experiments described here was initiated by the formation of a liquid droplet from a metal wire, as described previously(2). The wire was melted when it was overloaded by a high current from a discharge condenser inside a chamber in subatmospheric pressure. The sample is liquefied and liquid metal droplets at elevated temperature are produced. The radiating droplets formed then fall down in the chamber, being cooled during the time of fall.

The light emitted by the falling particles cooled by either method is recorded by stereophotography with two different narrow band filters on each objective. Finally, information about the temperature of the droplets may be inferred by scanning the two similar images with a photoelectric densitometer and using a calibrated curve of color density ratio vs temperature as a reference.

To enable color density ratio-temperature calibration, a sample of the metal wire was heated with direct electric current. The electric current was varied to give a range of temperatures which were measured by an optical pyrometer and the stereophotographic apparatus was used again to record a series of pictures of the heated wire at each temperature. Calibrated curves of resistivity-temperature found in the literature(3) were also used to determine the temperature of the sample and both the two methods of calibration gave identical results.

The position of the droplets during the flight was measured on the film with the aid of crosswires on the densitometer. The positions measured were converted to instants of time by photographing a scale which had been fixed to the chamber. In this way, plots of density ratio vs position were converted to the corresponding plots of temperature vs time.

3. Results and Discussion.

As is shown in Figure 1, the light emitted by the droplets gradually decreases in intensity, then abruptly increases, and smoothly decreases again. It has been shown that the point of sudden brightening coincides with the solidification of the radiating droplet(4).

A typical temperature-time curve to the droplets as that indicated by the arrow in the Figure 1 is presented in Figure 2. The continuous line denotes the purely radiative cooling the 400- μ diameter tantalum spheres should undergo in vacuum and certain approximations were made to estimate this curve. These are that the specific heat of the droplet does not change with temperature, and that the total emittance of the droplet is proportional to the temperature(3). We also consider the maximum temperature measured as the initial temperature of the radiating solid phase.

It should also be noted that the limit temperature T_L to the supercooling the liquid droplet undergoes is just the temperature before the droplet suddenly increases its intensity.

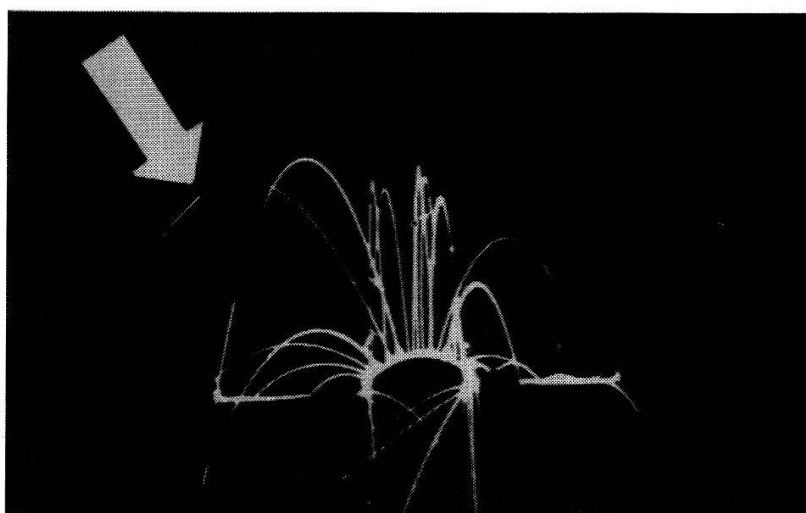


Figure 1. Photographic record of the light emitted by tantalum droplets falling in helium at 600 torr. Droplets fall without obstruction. The arrow indicates the abrupt brightening of the path of fall where the liquid-solid transition occurs.

This method offers almost ideal conditions for investigating nucleation in condensed phases at high temperatures because the relative small particle size minimizes the probability of heterogeneous nucleation. As a result, the sudden brightening has been observed repeatedly in metals such as W, Ta, Mo, and Nb.

The temperatures at the jumping have been determined and the fractional supercooling, related to the melting temperature T_M of the metals, is $(T_M - T_L)/T_M$. It thus appears that Turnbull and Cech's observation that the attainable degree of supercooling in a molten metal of about $0.18T_M$ should not be regarded as a firm limit. Singh and Holz have modified the free energy of nucleus formation in the "classical" theory and estimated theoretically an amount of supercooling $\Delta T = 0.56T_M$ which seems an overestimation of T_L .(8,5,1)

From the "classical" theory the jumping in the temperature is caused by exothermic solidification and at first sight, it would appear that a thermal jumping is inevitable since the large supercooling does not prevent the attainment of T_M upon release of the latent heat. However, such a kind of mechanism provides a time of solidification large and, until internal solidification is completed, the temperature should not fall rapidly as for a radiation-cooled sphere(6). This is not in agreement with our results.(See Figure 2)

The adiabatic theory of nucleation(7) provides a quantitative estimate of the supercooling $\Delta T \gtrsim 0.40T_M$ to the metals used in our experiments. Moreover, this model suggests the solid must appear at temperatures larger than that of the liquid nucleated but lower than T_M . Assuming the droplet is completely solidified at this temperature, the temperature of the surface must immediately begins to fall, as is observed.

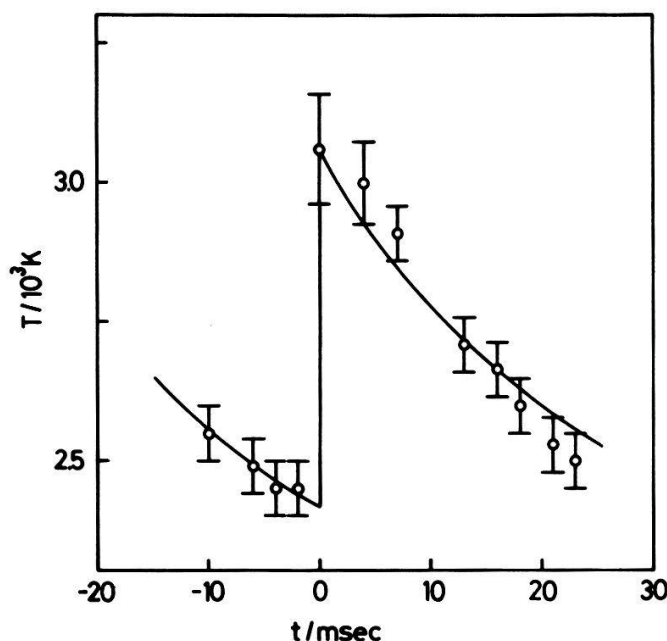


Figure 2. Typical temperature-time curve obtained to the cooling of Ta droplets. Continuous line corresponds to purely radiative cooling of 400-μ diameter Ta spheres. See the text to the assumptions used.

4. Conclusions.

It has been demonstrated that fundamental informations about the nucleation of metal droplets can be obtained by the technique of dendritic crystal growth coupled with a stereophotographic method in which photographic density is calibrated against temperature. The measured cooling rates in the vicinity of the solidification "point" to the metal droplets present the following characteristics: (i) the temperature does not form a plateau but, instead, immediately falls, producing a pointed trace; and (ii) dT/dt is the same as that expected for radiative cooling of a solid microsphere. The presented classical and adiabatic nucleation analysis show that the nucleation process may be considered as an adiabatic one.

Acknowledgements: It is a pleasure to thank the skillful assistance of Mr. Rossier with the photographs, and are also acknowledged the valuable support from the Fonds National de la Recherche Scientifique and Conselho Nacional de Desenvolvimento Científico e Tecnológico.

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Interface shape effects on the subcritical destruction of the superconducting state along a wire.

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Abstract: The theoretical description of the longitudinal propagation of a normal phase along a wire takes into account the latent heat absorbed by the superconducting to the normal state phase transition. The rate at which latent heat is absorbed depends on the separating boundary shape between the normal N and superconducting S phases and on the normal phase longitudinal propagation velocity. This paper compares the cases of a non planar or a planar separating interface between the N and S phases. It is shown that the best overall agreement between the theoretical and experimental data is obtained using a non planar separating boundary.

1. Introduction

Depending on the circulating electrical current intensity and on the efficiency with which heat is transferred to the cooling bath, the creation of a normal nucleus somewhere along a superconducting wire can result in the quenching of the superconducting state[1]. A successful theoretical model describing this destruction process must take into account the proper wire (geometry, electrical insulation, etc) and the proper bath (possible transient phenomena in the heat transferred to the bath[2], etc) characteristics.

2. Experimental apparatus

Different bare tin wires were immersed in a saturated normal or superfluid helium cooling bath. The current along the sample was supplied using a fast and stable current amplifier[3] and a pulsed local magnetic field nucleated a normal phase if no spontaneous creation of a normal nucleus occurred. The normal zone propagation velocity was deduced monitoring the voltage between two points along the wire.

3. Theory

A theoretical normal zone propagation velocity V is deduced solving the

heat equations describing the temperature profile along the wire[1]. The wire is divided into three parts: the normal N and superconducting S regions for which the wire cross section is completely in one state and the transition T region in which the phase transition from S to N occurs[4]. The temperature profile along the wire is calculated assuming a wire constant cross sectional temperature[1]. The differential heat equation describing the temperature profile is:

$$Q + K \frac{\partial^2 \Theta(z,t)}{\partial z^2} = C \frac{\partial \Theta(z,t)}{\partial t} + H(z,t) \quad (1)$$

where Q is the Joule heat released per u. vol., θ the temperature relative to the helium bath, z the longitudinal position, t the time, K the thermal conductivity, C the heat capacity and H the rate of heat transferred to the cooling bath per u. vol.

Equation 1 is simplified to a one dimensional second order differential equation using a moving coordinate[1]. The heat released to the bath is[4]:

$$H(z,t) = \frac{2}{a} \Theta(z,t) \left[h + \alpha \frac{\partial \Theta(z,t)}{\partial t} \right] \quad (2)$$

where a is the radius ($a = 0.15\text{mm}$) and h and α are respectively the steady and transient heat transfer coefficients, h being deduced by fitting the theoretical minimum electrical current (minimum current below which no destruction of the superconducting state occurs) to the experimental one, and α is neglected for a superfluid helium bath[5]. The values of h and α are listed on Table 1.

The heat equation describing the heat fluxes balance in the T region is:

$$\frac{V L \Sigma}{\pi a^2} = K \left[\frac{\partial \Theta(z,t)}{\partial z} \Big|_{z \rightarrow z_s} - \frac{\partial \Theta(z,t)}{\partial z} \Big|_{z \rightarrow z_n} \right] - \delta_o H(z,t) \quad (3)$$

where L is the latent heat absorbed by the superconducting to normal state phase transition, Σ the S and N phases separating interface lateral area, z_s and z_n respectively the S - T and T - N boundary position and $\delta_o = |z_s - z_n|$ the T region length. Σ is for a non planar separating interface (i.e. $\delta_o \neq 0$; otherwise $\Sigma = \pi a^2$)[4]:

$$\Sigma = \frac{2\pi}{3V^2D^2} \left[\left(V^2D^2a^2 + 1 \right)^{3/2} - 1 \right] \text{ where } D = \frac{\mu_o}{\rho} \quad (4)$$

Table 1 Wires characteristics versus bath temperature T_b

Wire	h [W/m ² K]	α [J/m ² K ³]	ρ [Ω m]	T_b [K]
Sn-1	$1.3 \cdot 10^4$	0	$2.33 \cdot 10^{-8}$	1.28
"	2100	0.8	"	2.3
Sn-2	7120	0	$3.4 \cdot 10^{-9}$	1.28
"	$1.72 \cdot 10^4$	0	"	2.12
Sn-3	600	1.7	$6.46 \cdot 10^{-9}$	2.3
Sn-4	440	6.4	$1.12 \cdot 10^{-9}$	2.3
"	"	1600	"	3.5

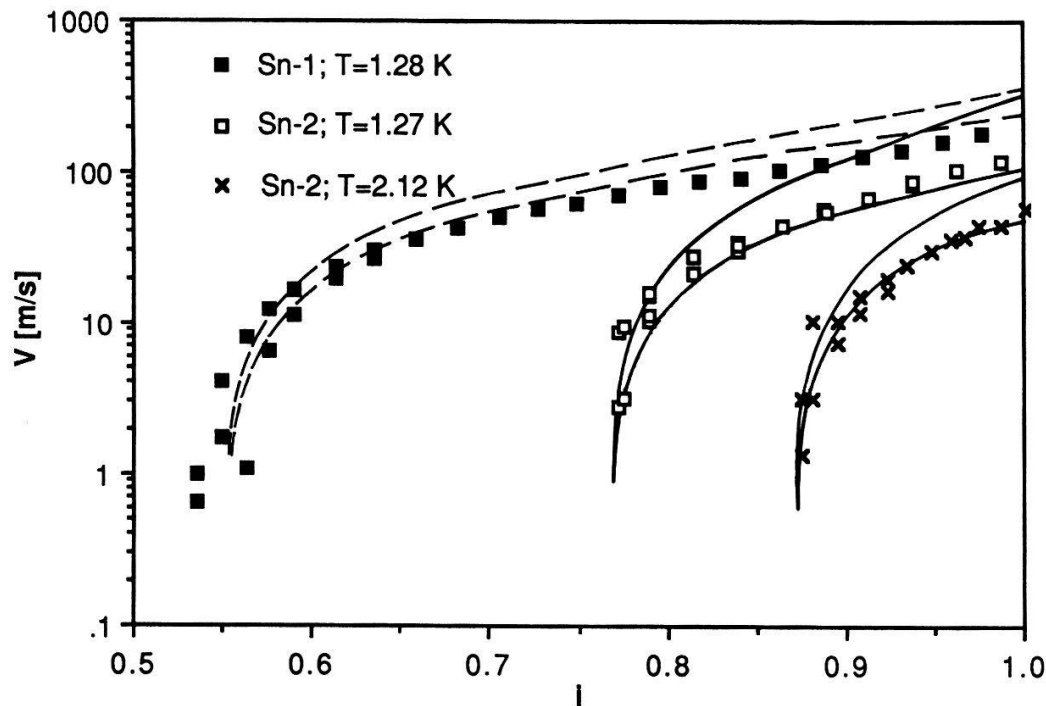


Fig 1 Measured and calculated normal zone propagation velocities versus normalized current in a superfluid helium bath. The upper theoretical curves assume a planar separating interface between N and S.

where ρ is the wire residual resistivity (Table 1) and μ_0 the vacuum permeability.

The calculation of the first derivatives that satisfies equation 3, permits to deduce the normal phase propagation velocity V as a function of the circulating electrical current and bath temperature.

4. Results

Figure 1 and 2 show the comparison between the experimental and theoretical data assuming planar and non planar separating interfaces. Figure 1 shows what is obtained with a superfluid helium bath. Using a planar separating interface between N and S, the calculated normal zone propagating velocities are higher, this effect being stronger for lower bath temperatures and wire electrical residual resistivities. The agreement between the experimental and theoretical data is improved if a non planar separating interface is assumed (Figure 1).

The data obtained with a normal helium bath is shown on Figure 2. As before, higher normal zone propagation velocities are observed for plane separating interfaces, the effect being diminished when compared with Figure 1. The agreement is somewhat better if a plane separating boundary is assumed, but a non planar separating interface is preferred in order to have the same theoretical model for a He-I or He-II bath.

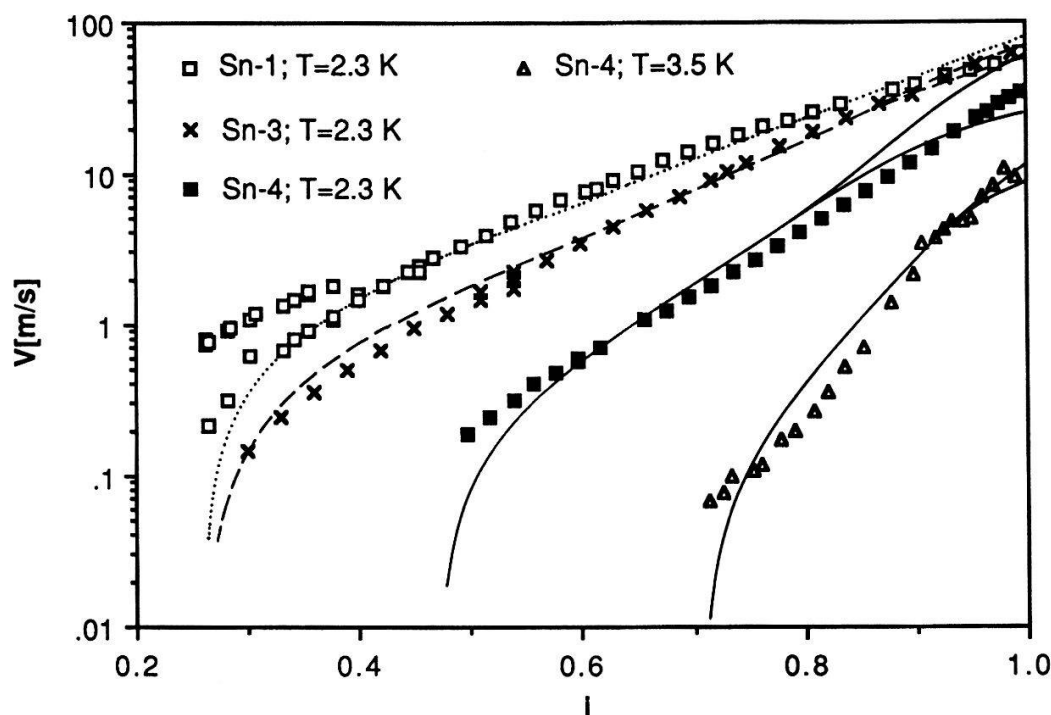


Fig 2 Measured and calculated normal zone propagation velocities versus normalized current in a normal helium bath. The upper theoretical curves assume a planar separating interface between N and S. For Sn-1 the two theoretical curves (with different N-S interface shape) are superimposed.

5. Conclusion

When the latent heat absorbed by the N to S phase transition is taken into account, a non planar separating interface is preferred with the present experimental configuration. For higher bath temperatures or residual wire resistivities, the difference between the theoretical results using a planar and a non planar separating interface diminishes. Once a non planar interface is chosen the agreement between the theoretical and experimental data is improved and the comparison between the two sets of data is an indirect means of studying heat transfer phenomena across a solid-He bath separating boundary[4-5].

This work was supported by the Swiss National Science Foundation.

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Mesure du diamètre moyen de bulles de gaz
par la méthode de l'écart-type

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Résumé.

La fluctuation d'intensité d'une onde ultrasonore transmise à travers de l'eau contenant des bulles est utilisée pour déterminer la taille des bulles. La relation entre l'écart-type du coefficient de transmission, la géométrie du volume de mesure et la taille de bulles a été établie par simulation numérique dans le cas de l'optique géométrique. Les mesures confirment la validité de la méthode.

Introduction.

Pour mieux contrôler l'aération des cultures de bactéries et pour étudier la formation des bulles, les chimistes ont besoin d'un appareil qui puisse mesurer localement le diamètre et la densité des bulles de gaz [1]. Cet article présente la méthode de mesure du diamètre qui a été développée pour cet appareil.

Le principe en est le suivant: Les bulles sont opaques aux ultrasons (US). Une onde US se propageant dans le milieu contenant les bulles voit son intensité réduite par celles-ci. Du fait du déplacement des bulles, différentes mesures i du coefficient de transmission des US donnent différents résultats T_i . L'écart-type σ caractérisant ces mesures est fonction de la taille et de la densité des bulles.

Par une série d'expériences simulées numériquement dans le cas de l'optique géométrique, la relation entre taille de bulles, σ et T , le coefficient de transmission moyen, a été établie. Cette relation a ensuite été généralisée aux US, qui sont nécessaires dans les milieux aqueux opaques que sont les bouillons de culture, puis testée avec succès lors de mesures US avec des bulles réelles.

Simulation numérique.

Les bulles sont traitées comme des sphères opaques placées aléatoirement dans un volume V_0 . V_0 est une boîte à fond carré de hauteur L traversée par un faisceau de lumière cylindrique et homogène de diamètre D_f définissant le volume de mesure V_m (fig. 1a). Une "mesure" consiste à calculer l'intensité I_i du faisceau ayant traversé une configuration i de sphères (fig. 1b).

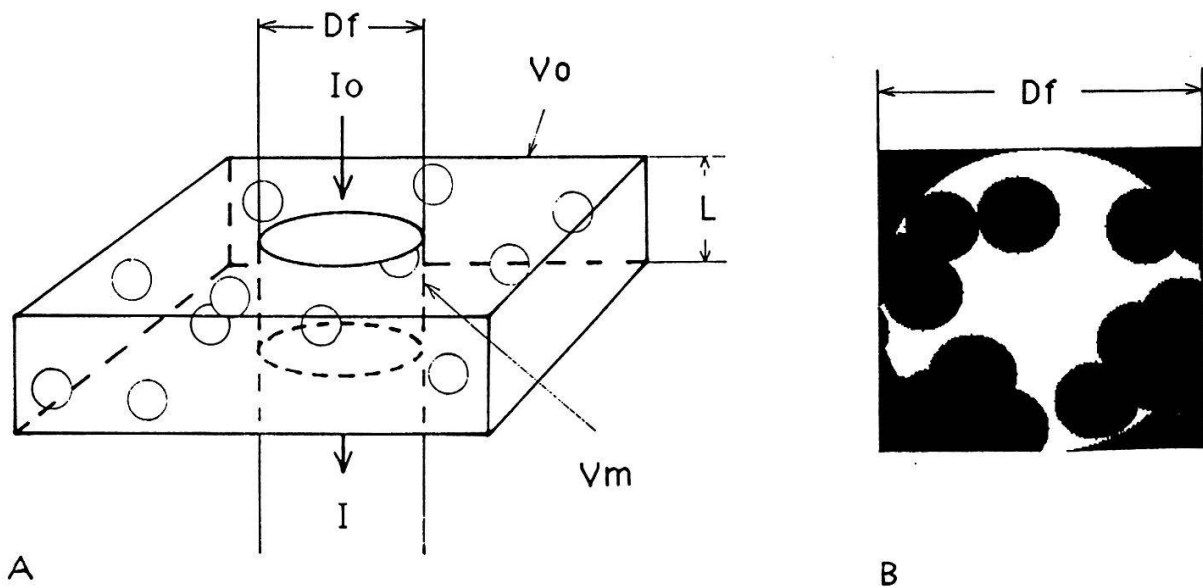


Fig. 1a: Géométrie de la simulation.

1b: Une configuration de sphères
vue par le faisceau lumineux.

Le volume V_0 est choisi de manière à ce que les sphères s'y comportent statistiquement comme dans un milieu infini, ce qui est vérifié lorsque T diminue exponentiellement comme (1). Cette dépendance est conforme aux observations [2]:

$$T = \bar{I}/I_0 = \exp(-C_n * S * (L-D)) \quad (1)$$

où: C_n est la densité de sphères, $S = \pi * r^2$ est la section géométrique des sphères et L est la longueur de mesure, $D = 2 * r$ est leur diamètre. Le terme $L-D$ décrit le fait que les bulles ne peuvent intersecter avec les membranes délimitant V_m (fig.3).

Après 10 000 "mesures" (5 h de CPU sur un VAX 8530) le coefficient de transmission moyen T est calculé ainsi que son écart-type. Cette procédure est répétée, pour une même taille de sphères, avec différentes longueurs de mesures L , afin de couvrir le domaine de $T = 0$ à $T = 1$. Finalement, différentes tailles de sphères donnent les courbes de la fig 2.

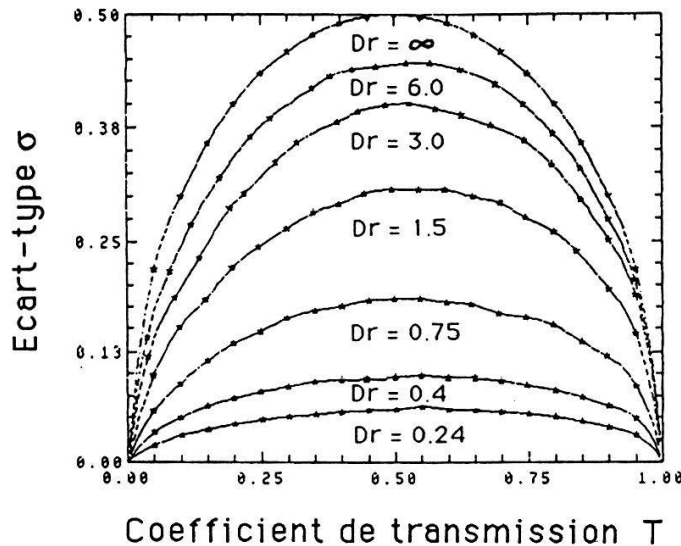


Fig. 2: Ecart-type du coefficient de transmission en fonction du coefficient de transmission, pour différents diamètres relatifs Dr des sphères. ($Dr = 1.5 \cdot D/D_f$).

Les résultats de la fig. 2 ont été obtenus pour des sphères de tailles égales occupant une fraction de 2% du volume total. Les études préliminaires de l'effet d'une distribution des tailles montrent que les grandes bulles, même en faible proportion, déterminent l'écart-type. L'augmentation de la fraction volumique cause un compactage des sphères et une diminution de σ . Les courbes de la fig 2. sont bien reproduites, pour $Dr \leq 3$, par une fonction de la forme :

$$\sigma(T, Dr) = \sqrt{T(1-T)} \cdot \sum_{k=1}^4 \left[(T-0.5)^{k-1} \cdot \sum_{\ell=1}^6 B(k, \ell) \cdot Dr^{\ell} \right] \quad (2)$$

Ce résultat d'optique géométrique peut être généralisée aux cas des US où les phénomènes de diffraction jouent un rôle important en remplaçant le diamètre géométrique D par le "diamètre efficace" calculé à partir de la section efficace.

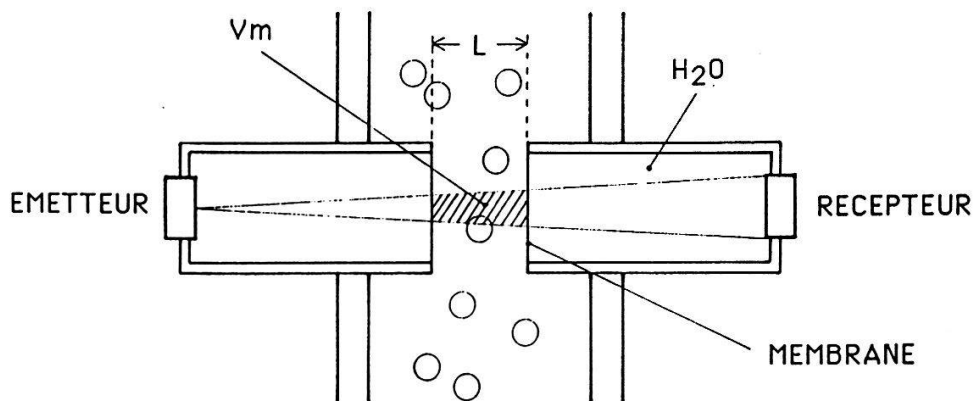
Vérification expérimentale.

Fig. 3: Schéma de principe de l'expérience.

Les mesures sont effectuées à l'aide d'impulsions d'US à 5 MHz dans une colonne à bulles contenant de l'eau de salinité de (NaCl) croissante pour réduire la taille des bulles. Celles-ci sont photographiées à l'endroit de la mesure US puis mesurées sur les photos. Les mesures US ont été interprétées sur la base de (2) sans l'usage d'aucun terme de correction ad hoc. Les résultats sont comparés sur la fig. 4.

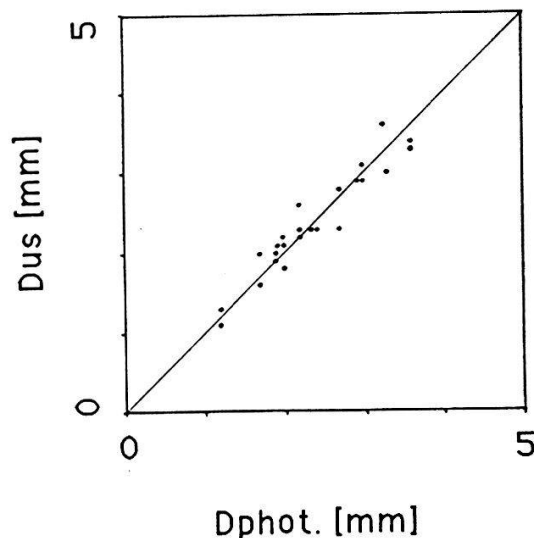


Fig. 4: Comparaison des diamètres de bulles mesurés par la méthode photographique et par la méthode de l'écart-type (Dus)

Conclusion

La méthode de l'écart-type constitue un nouvel outil de mesure sans contact des tailles d'objets dispersés[3].

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On the Theory of the Z-Pinch in a Dense Plasma

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According to some investigations, a dense D-T plasma column along which a sufficiently strong current is generated can serve as a fusion reactor (see e.g. [1], [2]). It was assumed in existing scenarios of such fusion generators based on the dynamical Z-pinch mechanism, that the pinch effect is produced in the gas having initially not too high density, see e.g. [3]. It follows, however, from elementary considerations [4] that the thermonuclear ignition can be achieved only if the initial plasma has a very high density. Assuming that the plasma confinement time coincides with its escape time in the radial direction, $\tau = \alpha r / v_{th}$ (r is the radius of the plasma cylinder, v_{th} is the ion thermal velocity, $\alpha \approx 10$ is a numerical factor [4], and defining the plasma radius from the Bennet condition $2nT = I^2 / 2\pi r^2 c^2$ i.e. $NT = W = I^2 / 4 c^2$, I is the current flowing along the plasma cylinder, n is the plasma density $N = n\pi r^2$, we can represent the parameter $n\tau$ in the form $n\tau = 3,2 n^{1/2} \alpha I$ where I is the current in MA. (The temperature T was assumed to be equal here to 10keV). Assuming $\alpha = 10$ we see that the Lawson criterion $n\tau \approx 10^{14} \text{cm}^{-3} \text{sec}$ can be fulfilled for $I = 10 \text{ MA}$ if the plasma density is equal to $n = 10^{24} \text{cm}^{-3}$. Such a plasma density can be indeed reached at the end of the plasma contraction if initial plasma density is equal to $n_0 = 10^{22} \text{cm}^{-3}$ and the ratio of the plasma density n at the end of the plasma contraction to n_0 is equal to about 10^2 , as it is indeed the case.

The purpose of this note is to show that the Z-pinch generated in a preformed solid state density plasma can lead to thermonuclear

ignition with substantial energy gains provided a current of a few MA could be generated there within the time plasma column is sustained by an external energy source, e.g. by a heavy ion beam. We will therefore use the following assumptions. 1) A beam of heavy ions produces a plasma column of a length l of a few cm. (The length l can not be too short lest the end plasma losses will prevent it from ignition). The heavy ion beams to be provided by SIS-18 at GSI/Darmstadt are just suitable for this purpose. For instance the beam of 40 GeV I^{20+} with energy 10^3 J can create a plasma channel of the length $l \approx 10$ cm in a frozen D-T mixture if one assumes for the range of ions in low Z materials the value 2 g/cm^2 [5]. 2) The current along the plasma column, which can be generated e.g. by two electrodes applied at its ends, rises to the value of the order of a few MA within the time the plasma column can be sustained by the heavy ion beam, i.e. within the time of the order of 100 nsec. It seems that possibility of providing such currents within the time 10^{-7} sec is within the reach of the modern Marx generator technology [2]. 3) The pinch remains stable within the contraction time which proves to be of the order of $10^{-7} + 10^{-8}$ sec. It seems that stability of the pinch is increased if the ion cyclotron radius corresponding to the magnetic field $H = 2I/cr$, is of the order of the plasma column radius (about 1 mm) coinciding with the radius of the heavy ion beam.

To describe the pinch contraction we will use model, time-dependent equations [4], [6] obtained as a result of space-averaging of hydrodynamical equations of the dynamical Z-pinch [6]

$$0 = 3 \frac{dNT}{dt} = -2\pi r \frac{H^2}{8\pi} \dot{r} - \frac{5NT}{\tau} - P_R + P_I = -4W_r \dot{r} - \frac{5W}{\tau} - P_R \delta \quad (1)$$

$$\frac{dN}{dT} = -\frac{N}{\tau} \text{ i.e. } \frac{dT}{dt} = \frac{T}{\tau} \quad (2)$$

The energy conservation equation (1) and the equation (2) describing outflow of plasma from the column were simplified under assumptions [4]: $I = \text{const}$ and $TN = W = \text{const}$. (dynamical Bennet equilibrium). Here τ is the plasma escape time ($1/\tau = v_{th}/l + v_{th}/\alpha r$), $P_R = 5 \cdot 10^{-24} T^{1/2} n^2 \pi r^2$ is the power loss per cm. due to radiation (the temperature T is expressed here and in the following in keV); $P_I = I^2 / \sigma \pi r^2$ is the plasma heating Joule rate per cm. of the plasma column, σ being the plasma conductivity. The

combination $-P_R + P_I$ can be written in the form $-P_R + P_I = -P_R \delta, \delta = 1 - I_{PB}^2/I^2$, $I_{PB} = 1$, 4MA being the Pease- Braginskii current. The solution of (1), (2) with initial conditions $r=r_0$, $T=T_0=W/N_0$ for $t=0$ is given by

$$\xi = \frac{r}{r_0} = (1-b) \left(\frac{T_0}{T}\right)^{5/4} + b \left(\frac{T_0}{T}\right)^2, \text{ for } \tau = \frac{\alpha r}{v_{th}} \quad (3)$$

where $b = 2 \cdot 10^{-6} W \tau_0^{3/2} \pi r_0^2 T_0^{3/2} \tau_0 = \alpha r_0 v_{th}^0$, ($v_{th}^0 = v_{th}(T_0)$). We will restrict ourselves here with the analysis of the case $b < 1$ corresponding to plasma cylinder collapse $r \rightarrow 0$ for $t \rightarrow t_1 \cong \tau_0$ with the temperature tending to infinity, $T \rightarrow \infty$, for $t \rightarrow t_1$. (For $r_0 = 1\text{mm}$, $n_0 = 10^{22}\text{cm}^{-3}$ this situation corresponds to currents $I > 6$, 4MA). Fusion energy q erg/cm released thereby in DT- mixture with $n_D = n_T = n/2$ can be now represented in the form

$$q = \frac{E}{4} \int_0^{t_1} \langle \sigma v \rangle n^2 \pi r^2 dt = \frac{EW^2 \tau_0 T_0^{1/2}}{4\pi r_0^2} \int_{T_0}^{\infty} F(T) dT \quad (4)$$

where $E = 17,6\text{MeV}$, $F(T) = \langle \sigma v \rangle T^{3,5} \xi(T)$, the rate $\langle \sigma v \rangle$ for the $D + T = \text{He}^4 + n + 17,6\text{MeV}$ reaction is defined as a function of T e.g. in [7] and the function $\xi(T)$ is given by (3). The energy spent in the process coincides approximately with the work $A = 4W \ln(r_0/r_f)$ performed by the current I for the plasma cylinder contraction (per cm. of its length) from r_0 till some final radius r_f . As the integrand $F(T)$ in (4) possesses a sharp maximum for some value T_m of the temperature T we will identify the ratio r_f/r_0 with $\xi(T_m)$ given by (3).

Thus the gain G corresponding to the process of a single plasma cylinder contraction can be defined as $G = q/4W \ln(1/\xi(T_m))$ with q defined by (4).

For $r_0 = 1\text{mm}$, $n_0 = 10^{22}\text{cm}^{-3}$ calculations lead to following values of q and G as a function of the current I

IMA	6,4	7	8	9	10	11
$q_{\text{erg/cm}}$	$3,8 \cdot 10^{14}$	$4 \cdot 10^{13}$	$2 \cdot 10^{13}$	$1 \cdot 10^{13}$	$0,9 \cdot 10^{13}$	$0,8 \cdot 10^{13}$
G	9,5	15	5	3	2	1,5

Thus, one can conclude from this table that the process described here may lead to substantial thermonuclear gains provided the technical problem of generating of currents of a few MA in the preformed solid density plasma column will prove to be feasible.

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Analyse de fonctions de réponse d'un mini-détecteur à scintillateur liquide NE-213

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Introduction :

Afin de déconvoluer la distribution des ions de recul obtenue avec un mini-détecteur NE-213 en vue de déterminer le spectre neutronique, il importe d'avoir des informations précises sur les fonctions de réponse de ce détecteur en fonction de l'énergie des neutrons incidents. Dans une certaine mesure, ces fonctions peuvent être estimées par des programmes de simulation numérique; cependant, celles-ci doivent être testées et ajustées à l'aide de mesures directes pour que l'on puisse se fier totalement aux résultats obtenus. La simulation numérique a été réalisée à l'aide du code "O5S" [1]. Ce code utilise la méthode Monte Carlo. Les mesures expérimentales ont été effectuées au SIN en utilisant des neutrons émis par une cible de lithium soumise au bombardement de protons de 16.4 MeV. En sélectionnant les 3 pics du spectre de la réaction ${}^7\text{Li}(p,n){}^7\text{Be}$ les fonctions de réponse ont pu être obtenues pour les énergies 14.0, 9.6 et 7.2 MeV. Le choix de l'énergie des protons de 16.4 MeV obéit au fait que le domaine d'énergie des neutrons couvert par le mini-détecteur pour nos études de couvertures de réacteurs de fusion est comprise entre 1 et 15 MeV environ.

Considérations expérimentales :

Le spectromètre consiste en une cellule en verre contenant le scintillateur liquide NE-213. Ses dimensions internes sont 13 mm de diamètre et 12 mm de longueur. Cette cellule est couplée à un photomultiplicateur (PMT) du type Hamamatsu R-1213. Ce PMT a été choisi pour sa bonne résolution temporelle et son faible bruit. L'ensemble de la configuration (cellule, PMT et l'embase) est logé à l'intérieur d'un tube à paroi mince en acier, étanche à la lumière, et dont les dimensions sont de 2.5 cm de diamètre et de 29 cm de longueur (cf. photo 1). Les dimensions réduites de ce spectromètre ainsi constitué, lui permettent d'être introduit à l'intérieur des couvertures pour des mesures in-situ, sans perturber d'une manière notable le comportement neutronique de l'assemblage.

Les expériences ont été effectuées en utilisant les neutrons émis par une cible de lithium naturel soumise au bombardement de protons de 16.4 MeV produits par le cyclotron PHILIPS du SIN. Pour le détecteur placé à 3.7 m de la cible de lithium dont l'épaisseur est de 0.76 mm, des spectres "tri-paramétriques", temps de vol (TOF), forme d'impulsion (PS) et hauteur d'impulsion (PH), ont été enregistrés (cf. fig.1). L'identification des événements détectés par le scintillateur NE-213 (neutrons ou γ) est réalisée par un circuit conventionnel de discrimination de forme d'impulsion utilisant la méthode de passage à zéro ("zero-crossing time"). Afin de détecter une éventuelle influence de la géométrie détecteur-faisceau de neutrons, les fonctions de réponse ont en outre été mesurées pour deux positions perpendiculaires du détecteur (relativement au faisceau de neutrons). L'enregistrement événement par événement des données a été conservé sur bande magnétique et traité sur le PDP 11/34 de notre laboratoire.

Détermination de l'énergie des 3 pics neutroniques:

Durant leurs parcours à travers la cible de lithium, les protons perdent un peu de leur énergie initiale. Cette perte d'énergie est estimée à 0.57 MeV. Ainsi, en moyenne, l'énergie des protons provoquant la réaction ${}^7\text{Li}(p,n){}^7\text{Be}$

est de 15.83 MeV. Ceci implique, après un calcul cinématique relativiste, une énergie de 14.15 MeV pour les neutrons observés à un angle zéro dans le référentiel du laboratoire. En se basant sur le spectre TOF (cf. fig.2) et le schéma simplifié des niveaux d'énergie du ^7Be (cf. fig.3), il apparaît que les niveaux supérieurs au niveau 7.21 MeV n'ont pu être excités de manière significative. En outre, on n'est pas certain que les autres niveaux ont été excités car la résolution du spectromètre en énergie ne permet pas de séparer les événements émis à l'état fondamental où au niveau 0.43 MeV, il en est de même pour les neutrons émis aux niveaux 6.73 MeV et 7.21 MeV.

En se basant sur les résultats de C.I.Batty et al [2], on a admis que le pic de neutrons le plus énergétique donné par le TOF consiste en 25% de neutrons émis à l'état correspondant au niveau 0.43 MeV et en 75% de neutrons émis à l'état fondamental. Par contre pour le 3^{ème} pic, nous n'avons aucune information sur les probabilités d'émission aux niveaux 6.73 et 7.21 MeV du ^7Be . Par conséquent, on a supposé que l'émission de ces deux niveaux est équiprobable. Ainsi, les énergies des 3 pics de neutrons données par la mesure du temps de vol sont estimées à : 14.0, 9.6 et 7.2 MeV.

Analyse des résultats :

Après normalisation, la comparaison des réponses calculée et mesurée pour le pic correspondant aux neutrons de 9.6 MeV montre un bon accord (cf. fig.5). Nous avons pris ce pic comme référence pour la comparaison car son énergie est bien définie. Le léger écart, qui se trouve vers la région où chute la fonction de réponse, s'explique par la résolution du mini-spectromètre NE-213 qui est de 10.4%. L'accord est tout aussi bon pour le pic des neutrons de 7.2 MeV, par contre il semble que l'énergie du pic des neutrons estimée à 14.0 MeV soit inférieure à cette valeur. Nous interprétons ce résultat comme une sous-estimation de la contribution des neutrons émis au niveau 0.43 MeV du ^7Be . Cette contribution devrait être supérieure à 25%.

La restauration du spectre des neutrons interagissant avec le mini-détecteur est effectuée à partir de la matrice de réponse calculée complètement par "O5S" et de la distribution des hauteurs d'impulsion (PH) déduite du bruit gamma. Cette opération a été réalisée à l'aide du programme FORIST [3]. La comparaison du spectre neutronique fourni par ce programme avec celui déduit des mesures de temps de vol fait apparaître d'importants écarts. La fig.7 montre les pics obtenus par FORIST nettement plus larges que ceux déterminés expérimentalement; aux énergies plus basses la divergence entre les deux spectres est beaucoup plus marquée. Ce désaccord nous semble provenir de FORIST puisque, comme le prouvent les fig.4, 5 et 6, le code "O5S" simule suffisamment bien les fonctions de réponse du mini-détecteur NE-213.

Conclusion :

La comparaison des 3 fonctions de réponse sélectionnées fait apparaître un bon accord entre les résultats numériques et expérimentaux, nous permettant ainsi de nous fier au code "O5S" pour la détermination complète de la matrice de réponse du mini-détecteur NE-213. Les réponses mesurées pour des positions du détecteur horizontale et verticale sont pratiquement les mêmes; ainsi la réponse du détecteur est quasiment indépendante de la géométrie détecteur-neutrons incidents. Enfin, une investigation plus approfondie est nécessaire pour déterminer si le programme "O5S" doit tenir compte ou non du tube d'acier qui assure l'étanchéité à la lumière du scintillateur NE-213.

Nous remercions Dr S.Jaccard du SIN, Dr R.Henneck de l'université de Bâle pour leur fructueuse collaboration et la mise à notre disposition de leurs installations d'acquisition de données.

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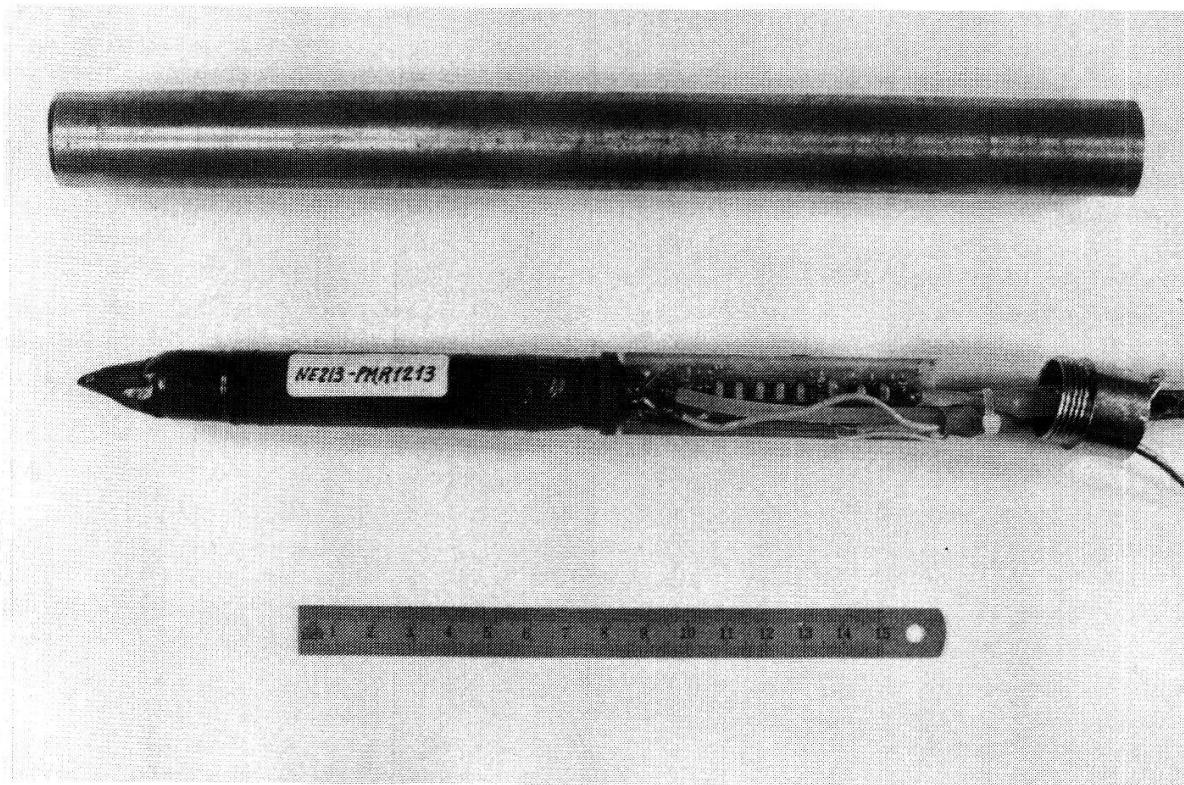


photo 1 : mini-détecteur à scintillateur liquide NE-213

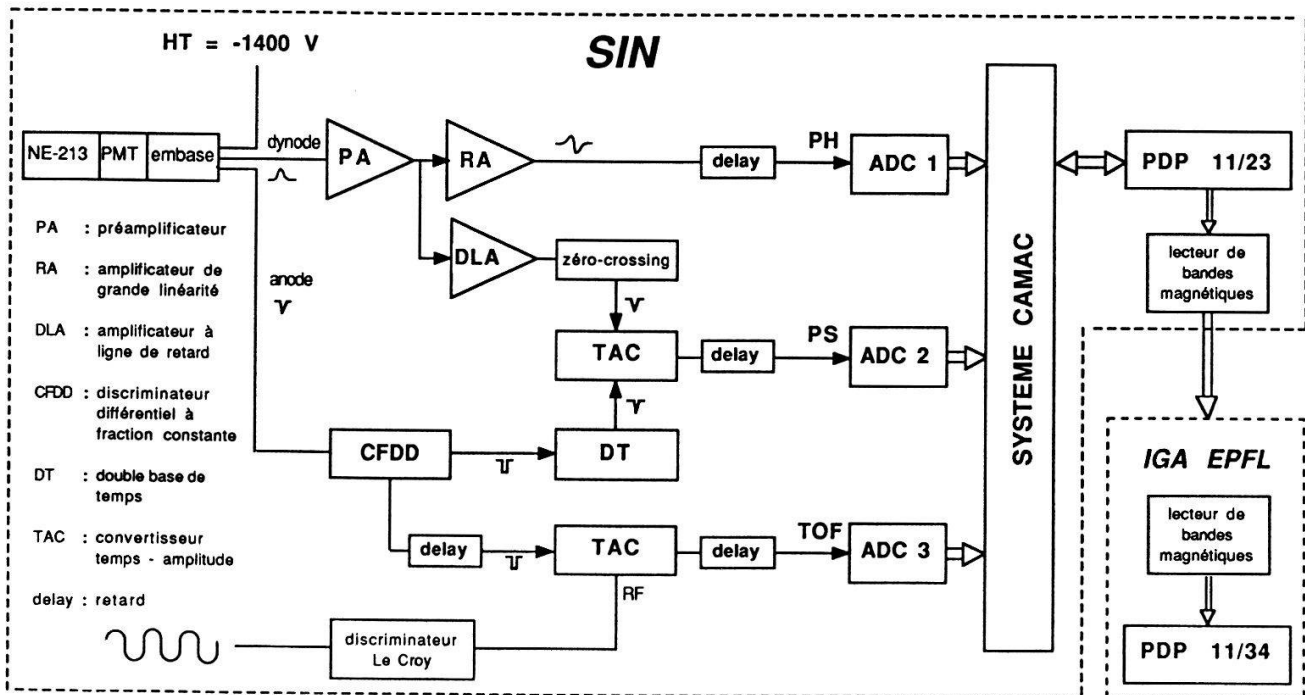


fig.1 : schéma du dispositif électronique d'acquisition tri-paramétrique

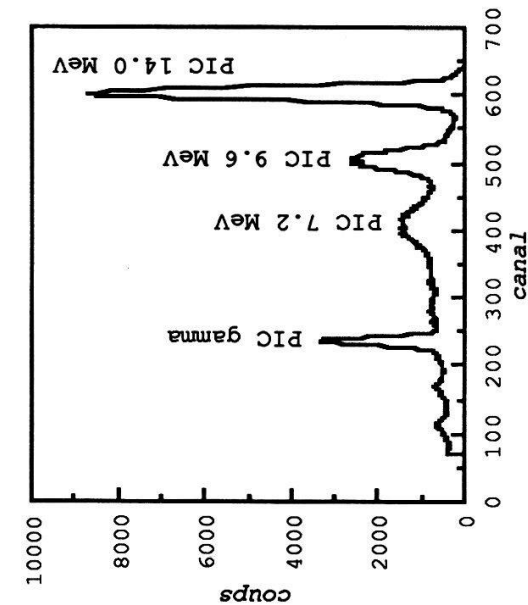


fig.2 : TOF (horizontal)

11.01	MeV
9.9	MeV
9.27	MeV
7.21	MeV
6.73	MeV
4.57	MeV
0.4292	MeV

fig.3 : niveaux d'énergie du ^7Be

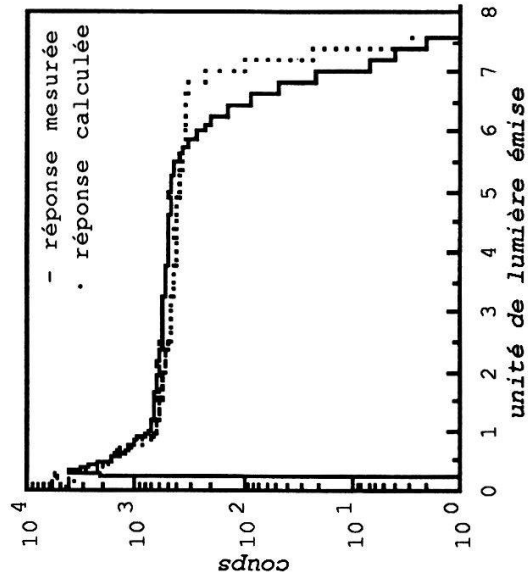


fig.4 : PIC 14.0 MeV (horizontal)

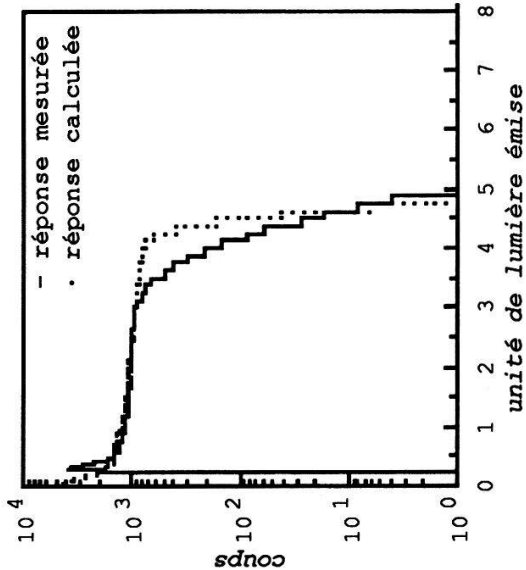


fig.5 : PIC 9.6 MeV (horizontal)

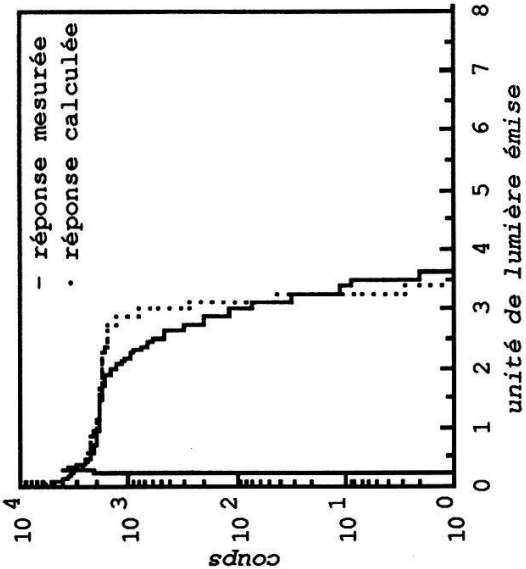


fig.6 : PIC 7.2 MeV (horizontal)

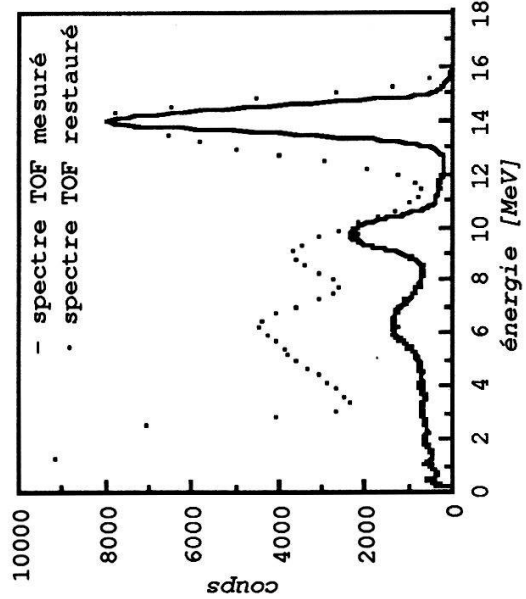


fig.7 : comparaison des spectres TOF

A Search for the Rare Decay $K^+ \rightarrow \pi^+ \mu^+ e^-$

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Abstract: A search for the lepton family number violating decay $K^+ \rightarrow \pi^+ \mu^+ e^-$ has been performed. We established an upper limit on its branching ratio of 1.1×10^{-9} at the 90 % C.L. Measurements have also been made for the decay $K^+ \rightarrow \pi^+ e^+ e^-$. A description of the measurement technique and some preliminary results are presented.

In the present framework of the Standard Model, lepton number conservation is strictly fulfilled.

The additive law has been observed for a long time, and over the years many experiments have given this experimental evidence:

Decay Mode	Branching ratio (90% confidence level)	Decay Mode	Branching ratio (90% conf. level)
$\mu^+ \Rightarrow e^+ \gamma$	$< 5 \times 10^{-11}$	$K_L^0 \Rightarrow \mu e$	$< 7 \times 10^{-9}$
$\mu^+ \Rightarrow 3e$	$< 2 \times 10^{-12}$	$K^+ \Rightarrow \pi^+ \mu^+ e^-$	$< 5 \times 10^{-9}$
$\mu^+ \Rightarrow e^+ \gamma \gamma$	$< 7 \times 10^{-11}$	$K^+ \Rightarrow \pi^+ \mu^- e^+$	$< 7 \times 10^{-9}$
$\mu^+ \Rightarrow e^+ \nu_e \nu_\mu$	$< 5 \times 10^{-2}$	$K^+ \Rightarrow \pi^- e^+ e^+$	$< 1 \times 10^{-8}$
$\mu^- \text{ Ti} \Rightarrow e^- \text{ Ti}$	$< 5 \times 10^{-12^*}$	$K^+ \Rightarrow \pi^- \mu^+ e^+$	$< 7 \times 10^{-9}$
$\mu^- \text{ Ti} \Rightarrow e^+ \text{ Ca}$	$< 2 \times 10^{-10\#}$		

Table 1: Some of the Experimental Evidence ⁽¹⁾
for Lepton Number Conservation;

Many of the theoretical models which extend the Standard Model, and by this extension describe new physics, lead to small violations of the law of lepton number conservation. For many of these models the K decays are good candidates for such observation.

In Brookhaven at the AGS we, the E777 collaboration, are doing a rare K decay experiment: we're looking for the decay $K^+ \rightarrow \pi^+ \mu^+ e^-$. At the same time we also collect data on the decay $K^+ \rightarrow \pi^+ e^+ e^-$.

The current upper limit for the branching ratio of the decay $K^+ \rightarrow \pi^+ \mu^+ e^-$ is $4.8 \times 10^{-9(2)}$. The same experiment got 41 candidates for the important decay $K^+ \rightarrow \pi^+ e^+ e^-$ - the only events of this process observed until recently.

In our experiment we are using an unseparated K^+ beam. Protons of 28 GeV/c are hitting a platinum target. With an acceptance of 6×10^{-4} str. GeV/c a positive 6 GeV/c K beam is selected by the bending magnets. The beam spill of the AGS is three seconds, out of which we are sensitive for about one second. The rates we normally run with are: with 5×10^{11} protons on target per pulse (which corresponds to about 5% of the machine capacity) we get about 10^7 K^+ , and in addition we have about 20 times more π^+ and protons. The beam halo rate, mostly μ^+ out of K^+ - and π^+ - decays, is about 1 % of the beam rate. At the end of the beamline is a 5-meter long decay volume in which 10% of the K's decay. With a detector acceptance typically

1 - 10 % for the different decay modes, we register about 10^5 K^+ decays crossing our apparatus per pulse.

A plan view of our set up with a hypothetical $\pi^+\mu^+e^-$ -decay is shown below.

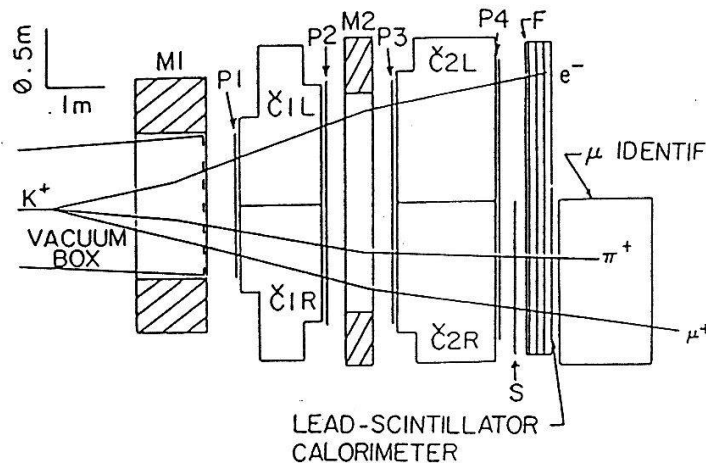


Fig. 1: Plan view of the E777 Detector

At the end of the decay volume, charge separation with the Magnet M1 is done. Partial-identification occurs in several steps. The first step is done with two Cerenkov counters C1 and C2. On the left side we want to be sensitive only to electrons. Here the Cerenkov counters are filled with hydrogen at atmospheric pressure. At the end of the left side there is a shower counter which allows us to distinguish π 's from e 's. Next steps: C1R and C2R have to be highly efficient for the detection of positrons and are therefore filled with CO_2 gas at atmospheric pressure.

Behind the shower counter on the right side a μ -identifier is installed to separate μ 's from π 's.

The spectrometer magnet M2 has two wire chambers installed P1, P2 in front and P3, P4 in the back.

Each MWPC has three signal planes with a 2-millimeter wire spacing. With this spectrometer configuration we get a momentum resolution of $\sigma_p = 0.01 \times p^2$.

For trigger purposes we have mounted two segmented walls of scintillation counters, F and S. To handle the enormous beam rate and halo in the middle of the detector, all the sensitive components have inefficient regions.

The detector is triggered for three different decay modes of the K^+ , each having three charged particles in the final state. Each trigger mode is built up on four different levels.

The first of the three modes is the τ -decay ($K^+ \rightarrow \pi^+\pi^+\pi^-$): this mode is used for calibrations and to check the efficiencies of the different components, as well as to compare the data obtained with our Monte Carlo program simulating the experiment. On the first level a coincidence between one charged particle on the left side and two charged particles on the right side in the F-scintillator wall has to be detected. The second level, a correlation of the right side F-counters (two particles) and the S-counter is asked for. Then levels three and four are just conditions on the hits in the different MWPC P1 - P4. The tau-decay is the dominant mode, about 10^5 per pulse, so this trigger is prescaled by a factor of 8192.

The second mode, the $\pi^+e^+e^-$ trigger mode, is also used for calibration and normalization purposes. In this mode we are also sensitive to the Dalitz decay, where the π^0 goes to e^+e^- and a γ which we do not observe. Also, this mode is prescaled by a factor of 8. Here on the first level the Cerenkov counters on the left side, C1L and C2L, have to see an electron and on the second level the Cerenkov counters on the right side, C1R and C2R, have to detect a positron. Again, on levels three and four the condition on the wire chambers have to be satisfied.

Finally, for the third decay mode $\pi^+\mu^+e^-$, we ask for an electron on the left side in the Cerenkov counters at the first level, two charged particles on the right side with the scintillators at the second level, and along with the wire chambers conditions we also want to have a minimum range of a track going into the μ -identifier.

Because we have both the τ and the π^+ -Dalitz samples, we are able to study the efficiencies of the different components of our detector. The measured efficiencies are shown in this table:

	C1	C2	Shower	μ -filter	Total
π^+	0.99	0.99	0.96	-	0.94
μ^+	0.99	0.99	>0.99	0.98	0.95
e^-	0.90	0.90	0.99	-	0.80
e^+	0.98	0.97	0.99	-	0.94

Table 2: Particle identification efficiencies

And in addition, we can also determine the probabilities of misidentification in the running environment. The results are summarized in this table:

	C1	C2	Shower	μ -filter	Total
π^- as e^-	0.002	0.002	0.14	-	6×10^{-7}
μ^- as e^-	0.002	0.002	<0.01	-	$<2 \times 10^{-8}$
e^+ as π^+	0.02	0.03	0.14	-	8×10^{-5}
e^+ as μ^+	0.02	0.03	0.14	<0.01	$<8 \times 10^{-7}$
π^+ as μ^+	-	-	-	0.04	4×10^{-2}

Table 3: Particle misidentification probabilities

We assume that the misinterpretation-probabilities are multiplicative, and we see that our particle identification system gives us the needed background suppression factors.

The data analysis and data reduction are done in different steps, beginning with the selection of tracks: one on the left side and at least two on the right side of the apparatus in an acceptable fiducial volume with a good vertex. This vertex is calculated, and by parameter S its quality is described. S is the minimum of the sum S_i^2 , where S_i is the distance of the tracks i to a common point. Next, we calculate the kinematical variables of the parent particle.

Finally, we do particle identification: all the responses of the different components of our detector have to agree according to the species of the daughter particle. For all these cuts and analyses, at every stage, we make comparisons between the Monte Carlo simulations and the data sample for τ - and π^+ -Dalitz decays, in order to understand and check our procedure. We find that the simulations and data are consistent.

For the final data reduction we proceed as follows: the τ -decay data are used as a template; distributions of position and angles at the production target are formed; for this sample the τ -events are required to have $S > 3$ cm: unambiguous particle-identification and a reconstructed invariant mass ± 15 MeV/ c^2 of the K^+ mass. (The standard deviation on the reconstructed K^+ mass from τ -events is $\sigma = 3.7$ MeV/ c^2 .) These distributions are then used as look-up tables for a likelihood comparison with the $\pi^+\mu^+e^-$ candidates.

Our results are shown as scatter plots of S versus the invariant mass of the reconstructed charged particle final state M. Figure 4 shows the plot for Taus. The signal region (for $M = 494 \pm 12$ MeV/ c^2 $S < 3$ cm) is also visible.

For the $\pi\mu e$ data the signal region for M has to be extended. (Higher Q-value). There are no events in the signal region. The nearest event with an acceptable S has a reconstructed mass of 467 MeV/ c^2 4.5 standard deviation away from the K^+ mass. Those events with low mass near

400 MeV/c² are consistent with misidentified Taus, followed by a decay of one or more pions. Events with higher mass and large S are due to random association of hits and tracks in an event.

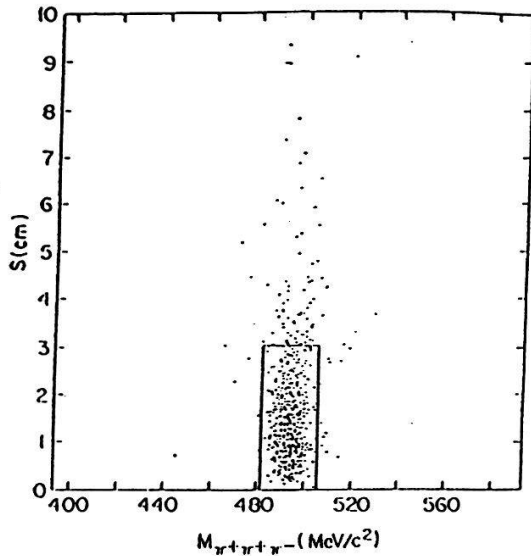


Fig. 2: Scatter Plot of S vs
Reconstructed Tau Mass

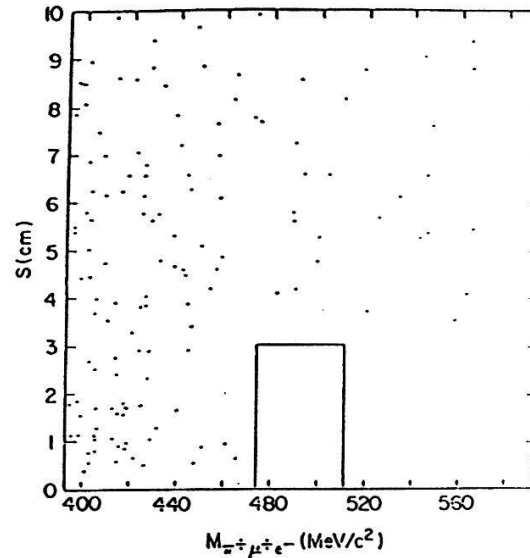


Fig. 3: Scatter Plot of S vs
Reconstructed $\pi\mu e$ candidates

To calculate the limit for the branching ratio of the $K^+ \rightarrow \pi^+\mu^+e^-$ decay we normalize to the π^+ -Dalitz decays.

We get a new upper limit on the branching ratio for the decay

$$K^+ \rightarrow \pi^+\mu^+e^- : 1.1 \cdot 10^{-9} \text{ (90\% CL)}$$

Since we don't see an event for the $K^+ \rightarrow \pi^+\mu^+e^-$ decay, we can also establish an upper limit on the branching ratio for the decay $\pi^0 \rightarrow \mu^+e^-$. With the appropriate acceptance and correction factors, we calculate an upper limit for BR ($\pi^0 \rightarrow \mu^+e^-$) of 7.8×10^{-8} (90 %CL). This branching ratio is the first to be reported directly by the group making the measurement, and it is comparable to the previously determined value.

All these values are based on the run taken in 1986/87. The newly obtained ratio for the $K^+ \rightarrow \pi^+\mu^+e^-$ decay is a factor of 4.4 improvement over the published value. This new limit can be used to set a lower limit on the mass of a gauge boson propagator for a new interaction, assuming standard model couplings; of 27 TeV/c⁽³⁾. For the run-period 87/88 we have improved our secondary beamline and the data taking. Due to these changes we have obtained approximately eight times more data which are now being analyzed. Without any event found, we will reach an upper limit of the $K^+ \rightarrow \pi^+\mu^+e^-$ decay of 1.5×10^{-10} . At the same time, we have collected about a thousand $\pi^+e^+e^-$ events. The scatter plot of these events is shown in Figure 5 as the reconstructed M_{ee} mass versus the $M_{\pi ee}$ mass. Events of an M_{ee} invariant mass less than 150 MeV/c² are mostly π^+ -Dalitz decays. The next Figure shows the invariant mass distribution for events with M_{ee} , the invariant mass of the leptons > 160 MeV/c². And in the next Figure the M_{ee} data obtained for $470 < M < M_{ee} < 515$ MeV/c² is shown. Superimposed are distribution assuming a scalar and a vector matrix element for this decay. It seems that the vector case is preferred. These results are preliminary and based on about 40 % of our data.

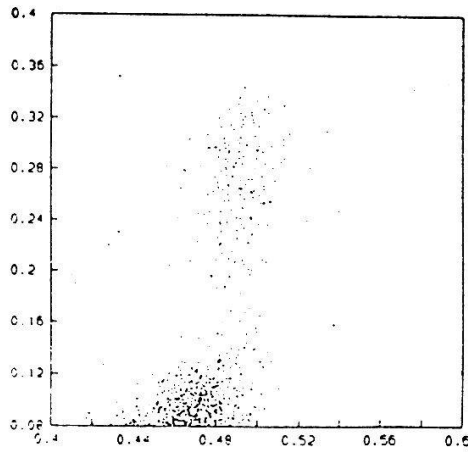


Fig. 4: $\rightarrow M_{\pi ee} [\text{GeV}/c^2]$
Scatter Plot of M_{ee} vs $M_{\pi ee}$

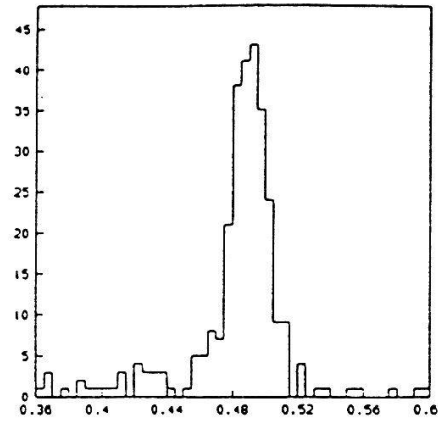


Fig. 5: $\rightarrow M_{\pi ee} [\text{GeV}/c^2]$
 $M_{\pi ee}$ Spectrum for $M_{ee} > 160 \text{ MeV}/c^2$

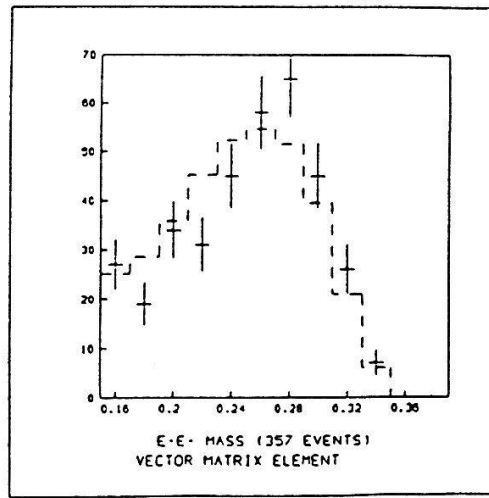
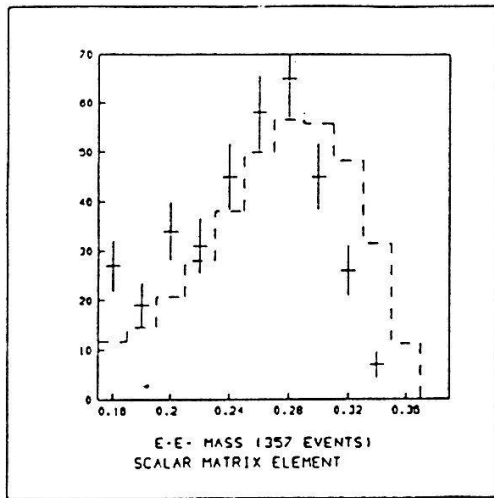


Fig. 6: M_{ee} Spectrum for: $470 < M_{\pi ee} < 515 \text{ MeV}/c^2$

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LAW OF CONSTANT PASSION AND INERTIA OF THE COSMIC DISTANCE

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Abstract : A law of constant passion (dim. TM^{-1}) : $t = \kappa m$ is introduced. For the gravitational value $\kappa = G/c^3$, this law amounts easily to Schwarzschild's radius formula and to Hubble's law of galactic recession. It gives way to a general relativistic scalar expression for a (variable) cosmological constant. The law is valid in Planck's Universe as well in Hubble's. Thus inertia is produced as the work of Planck's constant force F_P along the cosmic distance : $F_P r = mc^2$, with $F_P = c^4/G$.

1. Introduction

Besides the physical grandeur action, that is essentially the product of a time and a mass (more precisely, the scalar product of both of them vectorized by a velocity), it is relevant and meaningful to introduce the physical entity passion, as the quotient of a time by a mass. For almost 20 years now, it has been argued about a structural derevolution of Special Relativity when the differential system of passion $dx^i/p^i = dt/m$ is substituted to the action differential form (for one particle) $p_i dx^i - H dt$ [1].

2. Here a law of constant passion is considered, $t/m = x^i/p^i = \kappa$, in parallelism with Einstein-Planck law of constant action $ET = p\lambda = h$. Whereas h is a universal constant, κ is interaction depending [2].

3. It is clear that the simultaneous obedience to both laws of action and passion determines a constant length l_κ and a constant mass m_κ : $l_\kappa^2 = \kappa h$ and $m_\kappa^2 = h/\kappa c^2$.

4. The rest of this note is restricted to the gravitational interaction : $\kappa_G = G/c^3$. Then l_κ and m_κ are Planck's length and mass
 $l_P^2 = Gh/c^3$ and $m_P^2 = hc/G$.

Planck's time is determined on the light cone as $t_P = l_P/c$.

5. Planck's force

It is relevant also to define constant Planck's acceleration a_P and force F_P :

$$a_P = l_P/c_P^2 = c^2/l_P \quad (\text{Minkowski "centrifugal" type!}) \text{ and}$$

$$F_P = m_P a_P = m_P c^2/l_P = c^4/G.$$

Thus G acquires a more concrete meaning : it is essentially the inverse of Planck's constant force

$$F_P G = c^4$$

The magnitude of F_P is $1,21 \cdot 10^{44}$ Newton!

6. Planck's force is equal to Hubble's force

It is well known that (with r_H the actual radius of the Universe and M_H its actual mass) Hubble constant H is defined as the inverse the age of the Universe $t_H = r_H/c$ and the acceleration $a_H = c^2/t_H = cH$. Thus Hubble's force F_H is defined as

$$F_H = M_H a_H = M_H c/t_H = c/\kappa_H.$$

In accordance with the numerical values of H and M_H , one can admit that $\kappa_H = G/c^3$. That is to say that

$$F_H = F_P$$

i.e. the evolution of the Universe, from Planck's to Hubble's, (with a time ratio of $t_H/t_P = 10^{61}$ and consequently an action ratio of 10^{122}) has been made at constant passion. As mass grows uniformly with cosmic distance, there is no more need to appeal to an ad hoc missing mass!

7. Different forms of the law of constant gravitational passion $t = Gm/c^3$ are relevant :

a) Schwarzschild radius

On the light cone, $r = ct = Gm/c^2$.

Planck's length has the unique property to be simultaneously both Schwarzschild's radius r_S and Compton length λ_C of Planck's mass. For any other mass, r_S and λ_C differ. Reciprocally, for a given r , two different masses m_S and m_C can be ascribed, within a seesaw mechanism : $m_S m_C = m_P^2$ and $r_S \lambda_C = l_P^2$.

b) Inertia of the cosmic age

$$F_{Pr} = mc^2 \quad (1_P \leq r \leq r_H) :$$

inertia is associated to the work of Planck's force along the cosmic distance r (or cosmic age r/c).

c) Hubble law of galactic recession

As an immediate consequence of a)

$$Hr = Gm/c^2 t_H = (GM_H/c^3 t_H) (mc/M_H) =_d V_r$$

with an isotropic geometric effect of projection : $mc = M_H V_r$,
or equivalently : $r = ct = V_r t_H$.

d) A "cosmological constant" as a scalar form of Einstein equations for General Relativity (up to a factor 8π !)

Divide a) by r^3 :

$$\Lambda_r =_d r^{-2} = (G/c^4) mc^2/r^3 = F_P^{-1} \text{ density of energy.}$$

Thus $\Lambda_H = r_H^{-2} = 10^{-52} \text{ m}^{-2}$, in good accordance with the known constraints on Λ_H .

8. Newton law for gravitation $F_N = Gm_1 m_2 / r^2$

a) This law is natural for Planck's force :

$$F_P = Gm_P^2 / 1_P^2 .$$

b) F_N contains F_P ! (Newton-Einstein form) :

$$F_{NE} = F_P^{-1} E_1 E_2 / r^2 .$$

c) Possibility of quantization for F_N (!) :

$$F_N = F_P (m_1/m_P)(m_2/m_P)(1_P/r)^2$$

As $F_P 1_P^2 = Gm_P^2 = hc$, if there exists only integer multiples of h , then $F_P r^2$ or Gm^2 are also integer multiples of hc , and then :

$$r^2 = n 1_P^2 \quad \text{and} \quad m_i^2 = n_i m_P^2 \quad \text{and} \quad F_N = F_P (n_1 n_2)^{1/2} / n .$$

9. Newton law and Minkowski acceleration

Within Special Relativity, Minkowski has shown that an acceleration creates a curvature of the worldline, of magnitude c^2/ρ , where ρ is the radius of the hyperbola of curvature [3]. Then

$$c^4 = a_\rho^2 \rho^2 = GF_P ,$$

$$\text{i.e. } G/\rho^2 = a_\rho^2 / F_P .$$

Introducing a given mass m , one gets a gravitational acceleration

$$Gm/\rho^2 = m/M_H \cdot a_\rho^2 / a_H$$

a more precise form of a formula given by Milgrom [4], here obtained without any assumption of a revision of the law of inertia as Milgrom assumes.

10. Finally, in the frame of a theory of superunification, it is possible to conceive of other constants of passion, e.g. like the electromagnetic one $\kappa_{EM} = e^2/m^2 c^3$ (then $G_{EM} = e^2/m^2$ is mass depending, and the force $F_{EM} =_d c^4/G_{EM}$ presents no evident interpretation). One could also interpret the constant quark force F_q as a remnant of F_p after the break of symmetry, thus defining a constant $G_q =_d c^4/F_q$. These considerations are still too speculative to be reported here.

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IS GRAVITATIONAL ENERGY-MOMENTUM REALLY NON-LOCALIZABLE ?

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Abstract: It is shown that in two well known formalisms (Møller and Scherrer), the angular momentum of an insular system is tetrad dependent. From that follows the necessity to determine the tetrads uniquely. To this end one develops a theory founded on the notion of "torsion" (in the tetradic sense of the word). In comparison with some earlier similar, but purely formal attempts, the proposed theory has justly the advantage of being physically justified, which finally leads to gravitational energy-momentum localization.

0. Introduction

Nowadays most of the relativists consider that gravitational energy-momentum (GEM) is not localizable, because there is no physical argument supporting localizability (see for example [1], [2]). We think on the contrary that such an argument exists (sct. 1) and that it is consequently possible to develop a consistent theory of localizability (sct. 2), provided that we use f. ex. a tetrad formalism (it is true that GEM is not localizable in Einstein's formalism).

1. Tetrad-(in)dependence of the total energy-momentum and of the angular momentum

Consider an insular system described by a metric $g_{\mu\nu}(x)$ which satisfies the usual conditions at infinity. The tetrad components $g^{\lambda}_{\mu}(x)$ are connected with the $g_{\mu\nu}(x)$ by the relations:

$$g_{\mu\nu}(x) = \eta_{\alpha\beta} g^{\alpha}_{\mu} g^{\beta}_{\nu} \quad (1.1)$$

and are assumed to satisfy Møller's conditions at infinity [1]. The total EM complex of such a system is:

$$T_{\mu}^{\nu} \equiv \sqrt{-g} (\Theta_{\mu}^{\nu} + t_{\mu}^{\nu}) \quad \left(\text{with } \frac{\partial T_{\mu}^{\alpha}}{\partial x^{\alpha}} = 0 \right) \quad (1.2)$$

(Θ_{μ}^{ν} : matter EM, t_{μ}^{ν} : GEM). The t_{μ}^{ν} depend on the g^{λ}_{μ} and their first derivatives. In Møller's formalism, μ and ν are coordinate indices (though t_{μ}^{ν} is not a tensor, Møller's localizability condition is nevertheless satisfied). In Scherrer's formalism [3], μ is a tetrad index (T_{μ}^{ν}).

Now the question is to know whether the total EM of the system:

$$P_\mu \equiv \int T_\mu^0 d^3x \quad (1.3)$$

resp. the total angular momentum:

$$B^{\lambda\mu} \equiv \int (x^\lambda T^{\mu 0} - x^\mu T^{\lambda 0}) d^3x \quad (1.4)$$

depend or not on the tetrads (x^λ are coordinates which are Lorentzian at infinity). In the above mentioned formalisms, the P_μ are invariant under tetrad transformations which satisfy Møller's conditions at infinity. What's the matter with the $B^{\lambda\mu}$? We treat hereafter this question in Møller's formalism.

Consider a region D of the ordinary 3-dimensional space bounded by a surface S. Outside S, we leave the tetrads unchanged, but in the domain D, we vary the $g^{\lambda;\mu}(x)$ infinitesimally 1) consistently with (1.1), 2) so that the $g^{\lambda;\mu}(x)$ remain continuous on S. If the $B^{\lambda\mu}$ are tetrad independent, we then have $\delta B^{\lambda\mu} = 0$ identically for all these $\delta g^{\lambda;\mu}$. Consequently the corresponding Euler-Lagrange equations should be identities.

Let's apply f. ex. this procedure to the component $B^{0i} \equiv \int (x^0 T^{i0} - x^i T^{00}) d^3x$ in the particular case of a flat space-time. Here B^{0i} reduces to $-\int x^i T^{00} d^3x$. With the help of the Euler angles $\psi(x)$, $\theta(x)$ and $\varphi(x)$ ($\lim_{r \rightarrow \infty} \psi(x), \dots = 0$), the tetrads at each point of space-time may be written:

$$(g^{\lambda;\mu}) = \quad (1.5)$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\varphi \cos\psi - \sin\varphi \cos\theta \sin\psi & \cos\varphi \sin\psi + \sin\varphi \cos\theta \cos\psi & \sin\varphi \sin\theta \\ 0 & -\sin\varphi \cos\psi - \cos\varphi \cos\theta \sin\psi & -\sin\varphi \sin\psi + \cos\varphi \cos\theta \cos\psi & \cos\varphi \sin\theta \\ 0 & \sin\theta \sin\psi & -\sin\theta \cos\psi & \cos\theta \end{pmatrix}$$

Computing T^{00} ($\equiv \sqrt{-g} t^{00}$ in our case) is straightforward, but tedious (s. Møller's papers for the detailed expression of the t_μ^ν). The final result is ($\psi_{,i} \equiv \frac{\partial \psi}{\partial x^i}$, and so on):

$$T^{00} = \quad (1.6)$$

$$-\frac{1}{\kappa} \left\{ -\cos\psi \psi_{,1} \theta_{,3} - \sin\psi \sin\theta \psi_{,1} \varphi_{,3} - \sin\psi \psi_{,2} \theta_{,3} \right. \\ + \cos\psi \sin\theta \psi_{,2} \varphi_{,3} + \cos\psi \psi_{,3} \theta_{,1} + \sin\psi \psi_{,3} \theta_{,2} \\ + \sin\psi \sin\theta \psi_{,3} \varphi_{,1} - \cos\psi \sin\theta \psi_{,3} \varphi_{,2} - \sin\theta \theta_{,1} \varphi_{,2} \\ + \cos\psi \cos\theta \theta_{,1} \varphi_{,3} + \sin\theta \theta_{,2} \varphi_{,1} + \sin\psi \cos\theta \theta_{,2} \varphi_{,3} \\ \left. - \cos\psi \cos\theta \theta_{,3} \varphi_{,1} - \sin\psi \cos\theta \theta_{,3} \varphi_{,2} \right\}$$

The first of the 3 Euler-Lagrange equations for $J \equiv x T^{00}$:

$$\frac{\partial}{\partial x^\alpha} \left[\frac{\partial J}{\partial \psi_{,\alpha}} \right] - \frac{\partial J}{\partial \psi} = 0 \quad \text{gives} \quad (1.7)$$

$$-\frac{1}{\kappa} [-\cos\psi \theta_{,3} - \sin\psi \sin\theta \varphi_{,3}] = 0 \quad (1.8)$$

This relation is not an identity, therefore the angular momentum depends on the tetrads (the same is also valid in Scherrer's formalism). Because each component $B^{\lambda\mu}$ can have only a well definite value, it is then natural to admit that the tetrads have to be determined uniquely.

2. Determination of the tetrads. Theory

What are the supplementary conditions that the tetrads should satisfy? A thorough analysis¹⁾ leads to the conclusion that the tetrads have to be parallelized or, in other words, the "global torsion" (in the tetradic sense of the expression) is an extremum. Of course, the idea of parallelization is not new, but here, the alignment is not a simple mathematical procedure to "set in order" the tetrads. On the contrary, it appears now as a necessary physical consequence of the uniqueness of the angular momentum.

The non-alignment of the tetrads ("torsion") is locally characterized by the tensor $\tau^{\lambda}_{\mu\nu} \equiv D_{\nu} g^{\lambda}_{\mu}$ ($D_{\nu} \equiv$ covariant derivative). We easily obtain:

$$\tau^{\lambda}_{\mu\nu} \equiv D_{\nu} g^{\lambda}_{\mu} = f^{\lambda}_{\nu\mu} + g^{\lambda}_{\alpha} f_{\nu}^{\alpha\mu} + g^{\lambda}_{\alpha} f_{\mu}^{\alpha\nu} \quad (2.1)$$

where:

$$f^{\lambda}_{\mu\nu} \equiv \frac{1}{2} \left(\frac{\partial g^{\lambda}_{\mu}}{\partial x^{\nu}} - \frac{\partial g^{\lambda}_{\nu}}{\partial x^{\mu}} \right) \quad f^{\lambda}_{\mu\nu} \equiv g_{\mu}^{\alpha} f^{\lambda}_{\alpha\nu} \quad \text{etc.} \quad (2.2)$$

Let's write $\tau \equiv \tau^{\alpha}_{\beta\gamma} \tau_{\alpha}^{\beta\gamma}$ for the "torsion scalar". The parallelization is obtained by the variational principle with constraints:

$$\delta \int \tau \sqrt{-g} d^4x = 0 \quad (2.3)$$

with the constraints (1.1). We find for τ :

$$\tau = 3H_1 + 2H_2 \quad (H_1 \equiv f^{\alpha\beta\gamma} f_{\alpha\beta\gamma} \quad H_2 \equiv f^{\alpha\beta\gamma} f_{\gamma\beta\alpha} \quad H_3 \equiv f^{\alpha} f_{\alpha}) \quad (2.4)$$

The theory of this type of variational principle finally leads to the following result:

The $g^{\lambda}_{\mu}(x)$ have to satisfy the 16 equations:

$$a) \quad \eta_{\alpha\beta} g^{\alpha}_{\mu} g^{\beta}_{\nu} = g_{\mu\nu} \quad (10 \text{ equations}) \quad (2.5a)$$

$$b) \quad (\partial_{\alpha} + 2F_{\alpha})(F^{\alpha}_{\lambda\mu} - F_{\mu}^{\alpha\lambda}) - (\partial_{\lambda} F_{\mu} - \partial_{\mu} F_{\lambda}) = 0 \quad (6 \text{ equ.}) \quad (2.5b)$$

($\partial_{\alpha} \equiv g_{\alpha}^{\beta} \partial_{\beta}$ $\partial_{\alpha} \equiv$ Scherrer's covariant derivative)

$$c) \text{ and Møller's conditions at infinity.} \quad (2.5c)$$

¹⁾ This discussion is too long to be developed in this short paper. See a future publication (in preparation).

The 6 supplementary conditions (2.5b) are determined by the structure of τ (as a function of the H ; for the details of the calculations and the notations, s. in particular [4]). Note that, in this paper [4], we gave supplementary conditions which are different from (2.5b). But our argumentation was then purely formal and limited to the case of the weak field. In comparison with these relations, the equations (2.5b) have the advantage 1) to be physically well justified; 2) to result from general considerations which are not restricted to the case of the weak field.

The set of conditions (2.5a), (2.5b), (2.5c) should allow one to determine uniquely the 16 tetrad components $g^{\lambda}_{\mu}(x)$ of a given insular system, and consequently, to localize GEM (in a sense that we shall specify later).

In a future paper, we shall show that, in the post-Newtonian approximation, the above described procedure leads to a particularly simple result.

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Transformation to Normal Time for the Calculation of Poincaré Maps in a Closed Form

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Abstract

The calculation of Poincaré maps can be simplified by introducing a special rescaling of the flow vector field, namely the transformation to normal time. If that is done in an appropriate way, one can calculate the Poincaré map analytically.

1 Introduction

Oscillators with marked nonlinearity represent good models in various fields of physics. In many cases these systems have a smooth short-time behaviour but complex long-time dynamics. Mostly these equations cannot be solved in a closed form. On the other hand these systems can be effectively described by stroboscopic maps or Poincaré maps. For several problems it was shown that the dynamics of the continuous system is strongly correlated to the dynamics given by the corresponding map [2].

In this paper we present a method to calculate the parameters of a Poincaré map from the corresponding differential equation analytically. Recent studies by Wackerbauer et al. [1] have shown that it is possible to calculate a stroboscopic map from nonlinear ordinary differential equations in a closed form. However, in many cases the stroboscopic maps are too complicated for an effective description of the dynamic system. This is due to the coupling of frequency and amplitude of the oscillating system. This coupling is a general feature of nonlinear oscillators [3]. Due to this, Poincaré maps are independent of the amplitude frequency coupling and therefore for systems with a large amplitude frequency coupling sometimes essentially smoother and simpler than stroboscopic maps.

Recently it has been shown that for a large variety of oscillators an appropriate transformation, the normal time transformation, can be used in order to decouple amplitude and frequency. In this case stroboscopic maps are special Poincaré maps and are much less complicated. It should be now possible to calculate Poincaré maps by using algorithms designed for calculating stroboscopic maps and an expansion of stroboscopic maps with respect to the initial condition of the state variables should converge quickly. However this is not the case since the scaling function proposed in [4] was not continuous.

In this paper we present a new transformation for the decoupling of amplitude and frequency where the transformed flow vector field remains continuous. For linear oscillators amplitude and frequency are decoupled. Hence we propose a transformation that forces the angular velocity in phase space to be equal to that of a damped harmonic oscillator.

2 Transformation to normal time

For a two dimensional system of ordinary differential equations $\dot{\vec{x}} = \vec{F}(\vec{x})$ the angular velocity in phase space is given by

$$\dot{\varphi} = \frac{F_2 x_1 - F_1 x_2}{x_1^2 + x_2^2}.$$

For higher dimensional systems, x_1 and x_2 are two particular state variables that must be chosen conveniently. If it is possible to determine an appropriate Poincaré surface, it should also be possible to select the corresponding variables.

Multiplying the flow vector field by a scalar function $s(\vec{x})$ does not change the geometry of the trajectories. Choosing $s = 1/|\dot{\varphi}|$ one yields a constant angular velocity for the rescaled system. The disadvantage of that choice is that there is a singularity at $\vec{x} = \vec{0}$. In order to calculate a Poincaré map it is only necessary to set the period of the system to a constant value.

Therefore we suggest to choose $s = |\dot{\varphi}_H/\dot{\varphi}|$, where

$$N_H = \frac{x_2^2 + \gamma x_1 x_2 + \omega^2 x_1^2}{x_1^2 + x_2^2}$$

is the angular velocity of a damped harmonic oscillator with damping constant γ and frequency $\omega \cdot \sqrt{1 - (\frac{\gamma}{2})^2}$. To obtain a continuous scaling function one must choose γ and ω as follows:

$$\omega^2 = -\frac{1}{m} \left(\frac{\partial F_2}{\partial x_1} \right)_{\vec{x}=\vec{0}} \quad \gamma = \frac{1}{m} \left(\frac{\partial F_1}{\partial x_1} - \frac{\partial F_2}{\partial x_2} \right)_{\vec{x}=\vec{0}}$$

$$\text{with } m = \left(\frac{\partial F_1}{\partial x_2} - \frac{1}{2} \frac{\partial^2 F_2}{\partial x_2^2} \right)_{\vec{x}=\vec{0}}$$

Fig. 1 shows the effect of the transformation applied to the Rössler-System

$$\dot{x}_1 = -x_2 - x_3; \quad \dot{x}_2 = x_1 + ax_2; \quad \dot{x}_3 = b + x_3(x_1 - c).$$

3 Solving the rescaled equation

Using a numerical method like in [4] one can obtain the Poincaré map well approximated by a power series with only few nonzero coefficients:

$$x_{1_{n+1}} = \sum_{i,j=0}^{i+j=4} a_{i,j} x_{1_n}^i c^j$$

where x_{1_n} = n th cutting point of the trajectory with the Poincaré surface and $a_{i,j}$ represents a calculated coefficient.

The dependence of the map on x_3 is neglectible because the calculated coefficients are much smaller than the leading ones.

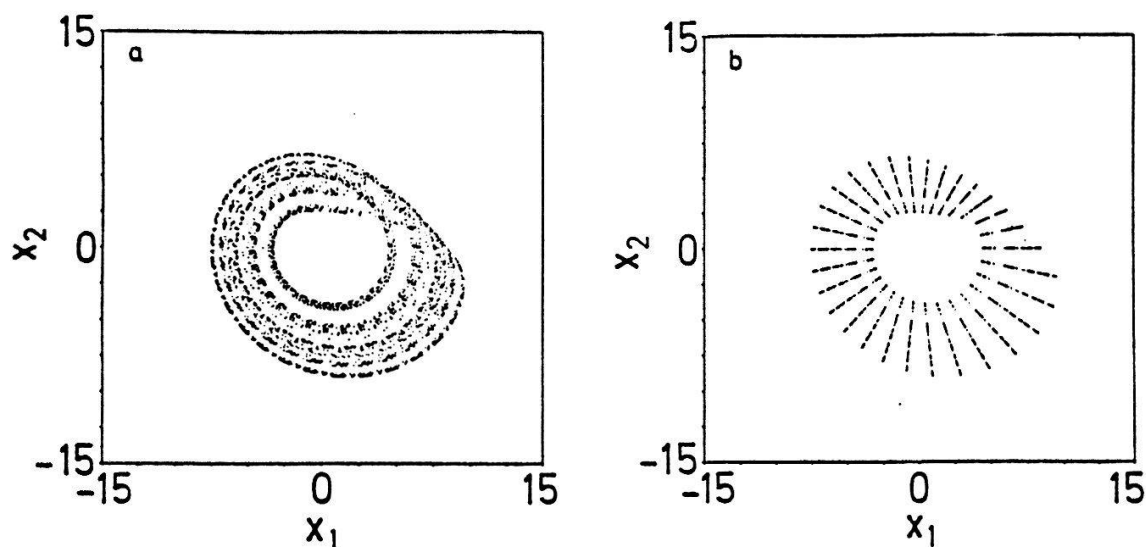


Figure 1: Discrete trajectories of the Rössler attractor projected in the (x_1, x_2) -plane. The left picture was calculated from the original equation with $a = 0.2$, $b = 0.2$, $c = 4.75$. The time between two points is $\Delta t = \frac{2\pi}{30}$. The right picture was calculated with the rescaled equation for the same parameter values by using the exact rescaling $s = \frac{x_1^2 + ax_1x_2 + x_2^2}{(-x_2 - x_3)x_2 - (x_1 + ax_2)x_1}$ and $\Delta t = \frac{2\pi}{30}(1 - 0.25a^2)^{-\frac{1}{2}}$.

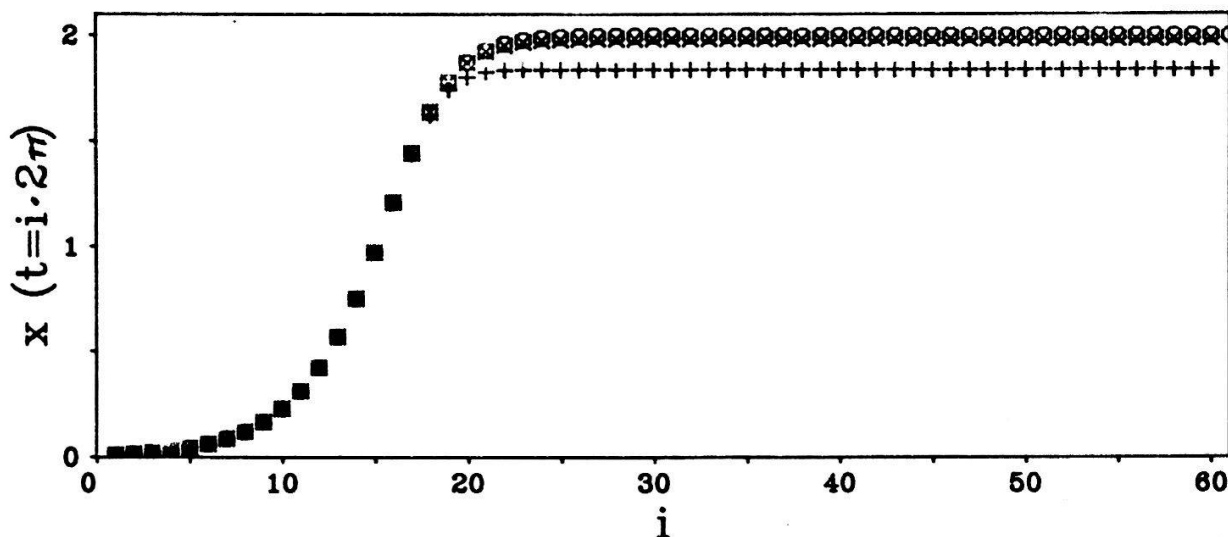


Figure 2: 60 numerical integrations over $\Delta t = 2\pi$ of the rescaled system of the van der Pol Oscillator $\dot{x}_1 = x_2$, $\dot{x}_2 = -x_1 + 0.1(1 - x_1^2)x_2$; (x): using the exact rescaling s ; (+, o): using the approximated $s = -1 + 0.1x_2 + 0.1(x_1 - 1)x_2 - 0.04(x_1 - 1)x_2^2 - 0.04(x_1 - 1)^2x_2^2$ with the expansion point $(1, 0)$; (+): setting $x_2 := 0$ after each integration; (o): $x_1 := \sqrt{x_1^2 + x_2^2}$ and $x_2 := 0$ after each integration.

$i_1 i_\mu$	a_{i_1, i_μ}	b_{i_1, i_μ}	c_{i_1, i_μ}
0 0	1.8213	2.6885	1.016
0 1	-5.5401	-1.8331	-0.089
0 2	3.2582	1.5343	0.490
0 3	-0.5292	-0.0383	
0 4	-0.0521		
1 0	-1.2041	1.6430	1.137
1 1	1.9245	2.1822	1.028
1 2	-0.0138	0.1769	
1 3	-0.3360		
2 0	0.1712	1.1403	0.615
2 1	0.1313	0.2795	
2 2	-0.4691		
3 0	-0.0442	0.1107	
3 1	-0.2769		
4 0	-0.0648		
Δs_m	$3.9 \cdot 10^{-3}$	$3.8 \cdot 10^{-2}$	$5.2 \cdot 10^{-2}$
Δs_l	$9.2 \cdot 10^{-3}$	$7.7 \cdot 10^{-3}$	$1.5 \cdot 10^{-2}$

Table 1: Coefficients of the Poincaré map for the Rössler system with $a = b = 0.2$

Another way is to use an analytical method that has already been developed [1]. For this algorithm it is necessary to represent the flow vector field as a polynomial. This can be reached by expanding s into a Taylor series around an appropriate point on the Poincaré surface. The deviation due to neglecting higher terms than second order are relatively small (Fig. 2).

We'd like to thank B. Buchberger, M. Singer and all the people at RISC Linz helping us to use Computer Algebra, and A. Hayd, M. Maurer and P. Meinke (MAN) for valuable discussions.

* Part of PhD thesis

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ADAPTIVE CONTROL OF CHAOTIC SYSTEMS

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Abstract: In order to describe the chaotic dynamics of a nonlinear system, a discrete map is reconstructed from the time series of an experimental system. The parameters of the map may depend on time. The map is a model for the dynamics of the experimental system. This model can be used in order to control the dynamics of the experimental system with small external perturbations, e.g. in order to get a special periodic dynamics or a special type of chaos. We argue that modelling and controlling can be done simultaneously.

1. Introduction

For a large variety of nonlinear oscillators higher order Fourier amplitudes fall off rapidly/1/. The dynamics of these oscillators can be approximated with high accuracy by a smooth interpolation between the extrema of the exact dynamics. The extrema of the dynamics can be calculated with special Poincare maps. The time between the extrema is the recurrence time of the Poincare map. Recently it has been shown, that these maps can be extracted from the time series of an experimental system/2,3,4/. Further it has been shown numerically/5/ and experimentally /6/, that these maps can be used for a control of the nonlinear system. In this paper we show that modelling and controlling can be done simultaneously.

2. Reconstruction of a map from an experimental time series

We assume, that N experimental data $\mathbf{x}_i^e$, where $i = 1, 2, \dots, N$ are continuously distributed in a certain range of the state space. By an appropriate rescaling of the coordinates of the state space $\mathbf{x}_i^e \rightarrow \mathbf{y}_i^e = \mathbf{S}(\mathbf{x}_i^e)$, where $\mathbf{x}_i^e$ are n -dimensional vectors and $\mathbf{S}$ is an n -dimensional function the data can be homogeneously distributed in the

unity cell of state space. For simplicity we restrict the following investigations to $n = 1$, but a generalisation to higher dimensional systems is straightforward. We assume that the experimental time series can be modelled by a map of type

$$y_{i+1}(y_i) = \sum_{k=1}^{\infty} b_k \sin(\pi k y_i) + F(\sigma_F^2, i) + F_c(i) + b_0 + b'_0 y_i \quad (1)$$

where y_i are one dimensional rescaled state variables, i represents time, b_k are the parameters of the model, $b_0 = y_{i+1}(0)$, $b'_0 = y_{i+1}(1) - y_{i+1}(0)$, and F is a uncorrelated random force. σ_F^2 is the variance of F . F_c represents perturbations which are applied onto the system in order to control it. We extract the parameters of the values b_k^e of the parameters b_k from the experimental data by a maximum likelihood estimation/6/:

$$b_k^e = \frac{2}{N} \sum_{i=1}^N (y_{i+1}^e - F_c(i) - b_0 - b'_0 y_i^e) \sin(\pi k y_i^e) \quad (2)$$

where the variance of b_k^e is

$$\sigma_{b_k}^2 = \frac{16\sigma_F^2}{\pi^2 N} \quad (3)$$

In order to investigate the quality of the model we use a F-test /7/. The model is accepted if the following relations hold:

$$Q = \frac{\sigma_m^2}{\sigma_F^2} = \frac{\frac{1}{N} \sum_{i=1}^N (y_{i+1}(y_i^e) + F_c(i) + b_0 + b'_0 y_i^e - y_{i+1}^e)^2}{\sigma_F^2} < f_{\alpha, N} \quad (4)$$

and

$$Q^{-1} < f_{\alpha, N} \quad (5)$$

where f is the f -distribution function /7/ and α is the confidence level. Now we rewrite the left side of Eq.(4)

$$\sigma_m^2 = \frac{1}{N} \sum_{i=1}^N (y_{i+1}^e - F_c(i) b_0 - b'_0 y_i^e)^2 - \frac{1}{2} ((b_1^e)^2 + (b_2^e)^2 + \dots) \quad (6)$$

Eq.(6) illustrates that Eq.(4) generally remains valid if some small parameters are set to zero. The decision which of these small parameters can be neglected depends on further information on the system or can be done by using more data. It can be easily shown, that the values b_k^e are independent of F_c .

3. Control of chaotic systems

In order to control the system we define an goal dynamics

$$w_{i+1} = G(w_i) \quad (7)$$

where w_n represents a state of the experimental system, and G is a real function. The goal of the control is to get $y_i = w_i$. This can be done by $F_c(i) = -\sum_{k=1}^{\infty} b_k \sin(\pi k w_i) - b_0 - b'_0 w_i + G(w_i)$, if $y_i = w_i$ is a stable solution of Eq.(1)/8/.

4. Numerical example

In order to investigate the control of a chaotic system we use a logistic map/9/

$$x_i^e = ax_i^e(1 - x_i^e) + F(\sigma_F^2, i) + F_c(i) \quad (8)$$

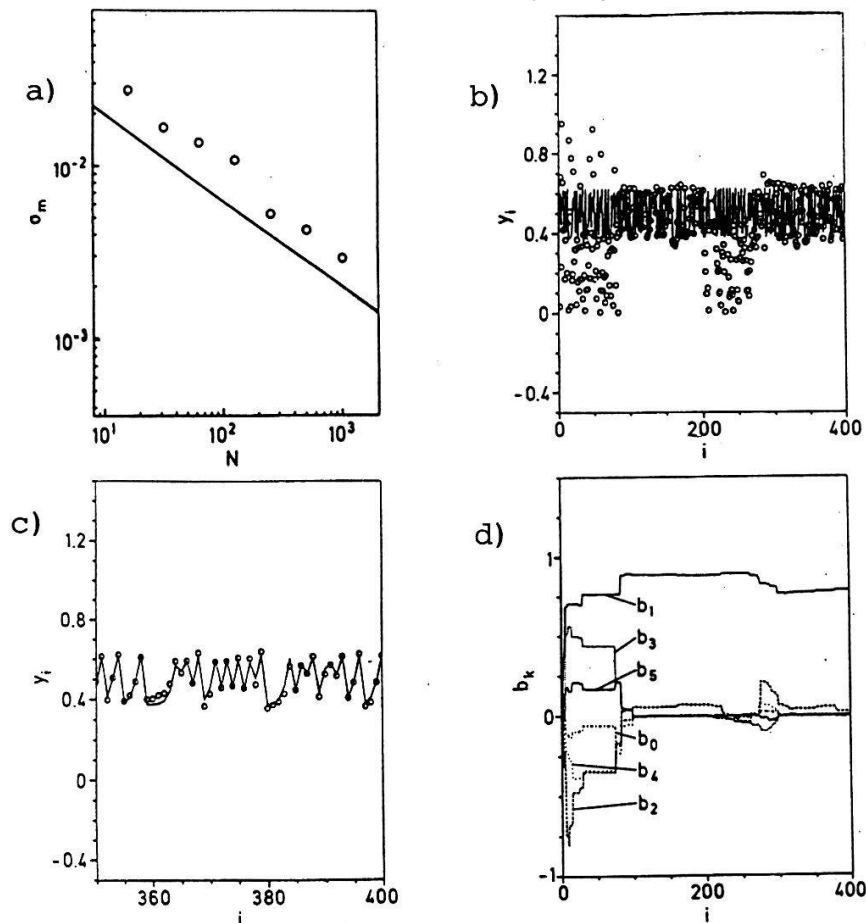


Fig. 1 Control of the logistic system: Fig. 1a the numerical (o) and the theoretical (-) value of σ_{b_k} versus N ($\sigma_F = .05$), Fig.1b,c the dynamics of the controlled system (o) and the goal dynamics (-) versus time ($\sigma_F = .01, N = 100, b=4$), Fig. 1.d the parameters of the model versus time, where $S = 4(x_i^e - .375)$

and the following goal equation

$$\begin{aligned}w_{i+1} &= 4(z_{i+1} - .375) \\ z_{i+1} &= bz_i(1 - z_i)\end{aligned}\tag{9}$$

Eq. (9) shows that the aim dynamics is closely related to the dynamics of a logistic map. For $b = 4$, the goal dynamics is chaotic.

Fig. 1a illustrates the relation between the variance of the estimated parameters and the number of data N . There is a good agreement with Eq. (3). The parameters of the model are extracted from the data in the range from $i - N$ to i . Fig. 1b shows the control of the logistic system Eq.(8). For $0 < i < 200$ a is set to 3.8 and the dynamics of the unperturbed system would be chaotic. Afterwards the unperturbed system would have a periodic dynamics, since a is set to 3.3. Fig. 1b and Fig.1c illustrate that it is not possible to control the logistic system directly after a sudden change of the parameters. But after a delay which is approximately equal to the number of data N (Fig. 1d) a control is possible again (Fig.1c). Further investigations show that no control of the dynamics is possible if N is too small, probably due to the uncertainty of the parameters of the model (see Eq.(3)).

A generalisation of these methods for systems which can only be modelled by differential equations is straightforward.

I acknowledge H.Haken, E. Lüscher, and O. Wohofsky for fruitful discussions and for continuous support.

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Description of the Dynamics of Nonlinear Extended Systems by Iterative Maps

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Abstract

The principle of iterative maps such as the stroboscopic map is well known for ordinary differential equations [1]. In this paper a generalization for systems with infinitely many degrees of freedom is presented.

1 Introduction

In nature we can find systems which can be described by a few degrees of freedom and such ones which have infinitely many degrees of freedom. An example for the first one is the classical mechanics of a masspoint, one for the last one is the dynamics of fields.

We want to handle with partial differential equations that can be written in the following form:

$$\frac{d}{dt}\vec{\Phi} = \sum_{\substack{r_1, \dots, r_m \\ 1 \leq \|\vec{r}\|_1 \leq p}} \vec{c}_{\vec{r}} \vec{\Phi}^{\vec{r}} \quad (1)$$

where $\vec{r} := (r_1, \dots, r_m)$, $r_i = 0, 1, \dots$, $\|\vec{r}\|_1 := r_1 + \dots + r_m$, $\vec{\Phi}^{\vec{r}} := \Phi_1^{r_1} \cdot \dots \cdot \Phi_m^{r_m}$ and $\vec{c}_{\vec{r}} := (c_{1,\vec{r}}, \dots, c_{m,\vec{r}})$. The $c_{m,\vec{r}}$ shall be Operators. This form is equivalent to a system of partial differential equations using the following definitions:

- $\Phi_m := \Phi_m(t, x)$
- $c_r := c_r(\nabla_x)$

The system is described by a tuple

$$\vec{\Phi} := (\Phi_1, \dots, \Phi_m)$$

$$\vec{\Phi} = \vec{\Phi}(t, x)$$

where t is a scalar $\vec{\Phi}(t)$ represents the state of the system at t . In common, t is the time, but it can also represent a spatial variable. $\vec{\Phi}$ shall obey a system of differential equations. The summation starts with $\|\vec{r}\|_1 = 1$ in order to ensure that the system has a fixpoint at $\vec{\Phi} = \vec{0}$. We now want to calculate the map $J_{\Delta t} : \vec{\Phi}(t) \mapsto \vec{\Phi}(t + \Delta t)$

2 Method to calculate $J_{\Delta t}$

In order to calculate the map $J_{\Delta t}$ one has to represent the solution of eq.(1) in dependency on the initial conditions:

$$\vec{\Phi}(t) = N(t)\vec{\Phi}_0 \quad (2)$$

where $N(t)$ represents a nonlinear operation and

$$\vec{\Phi}_0 = \vec{\Phi}(t = 0)$$

We suppose:

$$\vec{\Phi}(t) = \sum_{\substack{n_1, \dots, n_m \\ 1 \leq \|\vec{n}\|_1 \leq \infty}} \vec{a}_{\vec{n}}(t) \vec{\Phi}_0^{\vec{n}} \quad (3)$$

The $\vec{a}_{\vec{n}}(t)$ are tuples of operators acting on the products $\vec{\Phi}_0^{\vec{n}}$ and depending on t . Putting eq.(3) into eq.(1) there follows:

$$\sum_{\substack{n_1, \dots, n_m \\ 1 \leq \|\vec{n}\|_1 \leq \infty}} \frac{d}{dt} \vec{a}_{\vec{n}} \vec{\Phi}_0^{\vec{n}} = \sum_{\substack{r_1, \dots, r_m \\ \|\vec{r}\|_1 = 1}} \vec{c}_{\vec{r}} \sum_{\substack{n_1, \dots, n_m \\ 1 \leq \|\vec{n}\|_1 \leq \infty}} \vec{a}_{\vec{n}} \vec{\Phi}_0^{\vec{n}} + \sum_{\substack{r_1, \dots, r_m \\ 2 \leq \|\vec{r}\|_1 \leq p}} \vec{c}_{\vec{r}} \sum_{\vec{j}_1, \dots, \vec{j}_{\|\vec{r}\|_1}} [\vec{a}_{\vec{j}_1} \vec{\Phi}_0^{\vec{j}_1}] \cdot \dots \cdot [\vec{a}_{\vec{j}_{\|\vec{r}\|_1}} \vec{\Phi}_0^{\vec{j}_{\|\vec{r}\|_1}}] \quad (4)$$

One must be careful when deducing equations for the $\vec{a}_{\vec{n}}(t)$ because it is not allowed to make commutations within the term $[\vec{a}_{\vec{j}_1} \vec{\Phi}_0^{\vec{j}_1}] \cdot \dots \cdot [\vec{a}_{\vec{j}_{\|\vec{r}\|_1}} \vec{\Phi}_0^{\vec{j}_{\|\vec{r}\|_1}}]$. By transforming this term the sum of all exponents of $\vec{\Phi}_0$, which is $\vec{j}_1 + \dots + \vec{j}_{\|\vec{r}\|_1}$ is unchanged. If a transformation can be found:

$$\vec{b}_{\vec{r}} \vec{\Phi}_0^{\vec{j}_1 + \dots + \vec{j}_{\|\vec{r}\|_1}} = [\vec{a}_{\vec{j}_1} \vec{\Phi}_0^{\vec{j}_1}] \cdot \dots \cdot [\vec{a}_{\vec{j}_{\|\vec{r}\|_1}} \vec{\Phi}_0^{\vec{j}_{\|\vec{r}\|_1}}], \quad \text{for all } \vec{\Phi}_0$$

one gets an algorithm to calculate the $\vec{a}_{\vec{n}}$:

$$\frac{d}{dt} \vec{a}_{\vec{n}} = \sum_{\substack{r_1, \dots, r_m \\ \|\vec{r}\|_1 = 1}} \vec{c}_{\vec{r}} \vec{a}_{\vec{n}} + \sum_{\substack{r_1, \dots, r_m \\ 2 \leq \|\vec{r}\|_1 \leq p}} \vec{c}_{\vec{r}} \sum_{\vec{j}_1 + \dots + \vec{j}_{\|\vec{r}\|_1} = \vec{n}} \vec{b}_{\vec{r}} \quad (5)$$

$\vec{j}_1 + \dots + \vec{j}_{\|\vec{r}\|_1} = \vec{n}$ causes the indices of $\vec{a}_{\vec{j}}$ to be smaller than those of $\vec{a}_{\vec{n}}$ because $\vec{a}_{\vec{0}} = \vec{0}$ and the original differential equation has a fixpoint at 0. Then one can construct the equation for $\vec{a}_{\vec{n}}$ from $\vec{a}_{\vec{1}}, \dots, \vec{a}_{\vec{n}-1}$ and calculate $\vec{a}_{\vec{n}}$. So the $\vec{a}_{\vec{n}}$ can be successively calculated.

3 Example: Nonlinear Diffusion

We have investigated a nonlinear diffusion equation which can be assumed to be a special case of eq.(1), where $V := \{R^l \mapsto R; \vec{x} \mapsto \Phi(\vec{x}); \vec{x} : l \text{ spatial coordinates}\}$

$$\frac{d}{dt}\Phi = \Delta\Phi - \gamma \cdot \Delta\Phi^2 \quad (6)$$

Fig.(1a) shows the comparison with the numerical solution.

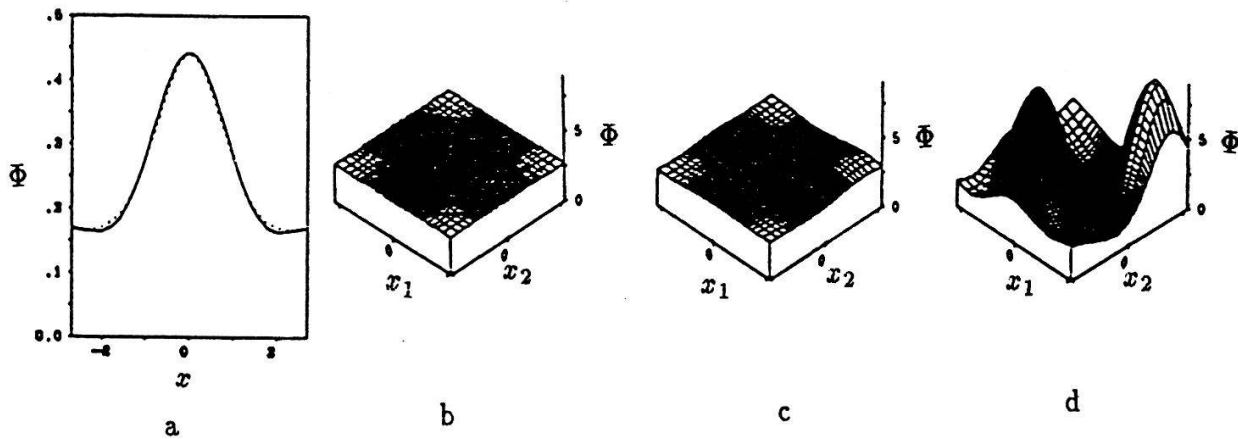


Figure 1: Density Φ vs. $\vec{x}$ represents the state of the system at a certain time t ; a: comparison with numerical simulation after 1 iteration with $t = 0.5$ and $\Phi_0 = 0.7 \cos(x)e^{-\frac{x^2}{9}}$ (— theory, ... simulation); b: initial condition for pattern formation¹, c: after 7 iterations, d: after 12 iterations; the parameters were $\gamma = 0.5$ and $t = 0.5$

1 The initial condition for the pattern formation was

$$\Phi_0 = 2.7 + 0.05 \text{random}(x)$$

where $\text{random}(x)$ is a function defined in the following way:

- $-1 < \text{random}(x) < 1$
- the value of $\text{random}(x)$ is generated by a random number generator.

4 Conclusion

Under certain conditions, namely those done in chapter 1, a partial differential equation can be analytically transformed into a stroboscopic map. This map allows a very efficient study of systems whose dynamics have a complex dependence on the control parameters. The calculation time is much smaller compared to pure numerical simulations/4/. The

difference to the calculations done by A. Hübler and R. Wackerbauer is that here we have to do with operators instead of normal coefficients.

We would like to thank A. Hübler, A. Hayd and M. Maurer for valuable discussion, P. Meinke and O. Wohofsky for continuous support.

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*part of Ph. D. thesis

PHONON INDUCED DELOCALIZATION NEAR THE MOBILITY EDGE
OF AN AMORPHOUS SEMICONDUCTOR

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Abstract : The electrical conductivity of an amorphous semiconductor is calculated using the selfconsistent transport equations proposed by Götze. The electron-phonon interaction used in the model produces a non-zero finite temperature conductivity even below the mobility edge.

The phenomenon of localization and the behaviour of the electrical conductivity σ in disordered materials is a fascinating subject. Götze and his collaborators have provided an approximate analytic approach for describing the breakdown of the electronic mobility at the mobility edge [1,2]. We have used the same approach in order to calculate the temperature and frequency dependent conductivity $\sigma(T, \omega)$ near the mobility edge in the conduction band of an amorphous semiconductor. $\sigma(0,0)$ goes to zero when the Fermi energy E_F goes to E_c , the mobility edge, and is zero below E_c [1]. At $T > 0$ the phonons delocalize the electrons : $\sigma(T,0)$ remains non-zero below E_c . In order to obtain this delocalization effect we find two points important : the phonons should couple to the electronic kinetic energy (the same coupling as in [2]), but the adiabatic approximation used in [2] has to be abandoned. Similar phonon induced delocalisation has been found [3] in a tight binding approach.

Our Hamiltonian [2] describes independent electrons of density n moving in a random static ion potential $U(\vec{r})$ and interacting with vibrational modes. The electron-phonon interaction reads (in the usual notation) :

$$H_{el-ph} = \sum_{\vec{q}, \vec{k}} V(\vec{q}) \rho_{Ion}(\vec{q}) \frac{k^2}{2m} c_{\vec{k}+\vec{q}/2}^+ c_{\vec{k}-\vec{q}/2} \quad (1)$$

The dynamic conductivity is given by [2] :

$$\sigma(\omega) = \frac{ie^2 n}{m} \left[\frac{1}{\omega + M(\omega)} - L(\omega) \right] \quad (2)$$

$$\text{with } M(\omega) = \int d^3 p |U(\vec{p})|^2 \int d\omega' S(\vec{p}, \omega') \phi_0(\vec{p}, \omega - \omega') \quad (3)$$

$$L(\omega) = \int d^3 p |V(\vec{p})|^2 \int d\omega' S(\vec{p}, \omega') \phi_1(\vec{p}, \omega - \omega') \quad (4)$$

The density and current relaxation functions, ϕ_0 and ϕ_1 , can again be expressed by the memory kernels M and L [1,2]. In order to solve the resulting non-linear equations for M and L we have approximated ϕ_0 and ϕ_1 by their large M form [1] and taken the electron-phonon coupling V to be small. The dynamic structure factor S is divided into its static part S_0 and an Einstein contribution $S(q, \omega) = S_0(q)\delta(\omega) + \phi(q)[\delta(\omega - \omega_0) + \delta(\omega + \omega_0)]$. When all phonon effects are neglected, the known [1,4] relation for the static resistivity $\rho \equiv -iM(0)$ is obtained :

$$(1 - A(E_F))\rho = v + o\left(\frac{1}{\rho}\right) \quad (5)$$

For a free electron like band model the quantity A (involving S_0 and U) increases when E_F goes down. Thus $\sigma = \rho^{-1}$ goes to zero when $E_F \rightarrow E_C$ ($A(E_C) = 1$) and remains zero below E_C .

The effect of lattice vibrations in (3,4) is to shift the frequency of the electronic correlators ϕ_0 and ϕ_1 by the phonon frequency ω' (equal to a single ω_0 in our Einstein model). Avoiding the adiabatic approximation this yields a hierarchy of equations, through which $M(\omega)$ and $L(\omega)$ are coupled to $M(\omega \pm n\omega_0)$ and $L(\omega \pm n\omega_0)$ for arbitrary n . Physically this means that the "conduction channel" at a given low frequency ω (e.g. $\omega = 0$), where strong disorder tends to immobilise the electrons, is coupled to higher frequency channels where the effect of disorder is less important. This mechanism yields the "delocalisation effect" seen in Fig. 1.

In order to get concrete results for $\sigma(\omega)$ with $\omega \ll \omega_0$ we have truncated the hierarchy by assuming that $M(\omega \pm n\omega_0)$ is relatively small for $n > N$ (the system is a reasonable conductor at high frequencies) and that at those frequencies the electron-phonon coupling has a negligible effect on M . For simplicity we chose $N = 1$, but higher order truncations would also be possible. As a result relation (5) is replaced by

$$\left[1 - \frac{A(E_F)}{1 + aF - ib\omega F} \right] F = v + o\left(\frac{1}{F}\right) \quad (6)$$

where $F(\omega) \equiv -iM(\omega)$ and a is proportional to the phonon intensity ϕ in the dynamic structure factor. The conductivity is then given by $\sigma(\omega) = F^{-1}(\omega) = \sigma'(\omega) + i\sigma''(\omega)$.

The delocalisation effect at $\omega = 0$ is easily seen in eq. (6) : when F increases ($E_F \rightarrow E_c$) the term aF in the denominator counterbalances the effect of A and prevents F from diverging. Figure 1 shows $\sigma(T, \omega = 0)$ for different values of a , corresponding to different "phonon temperatures" (the electronic system is treated at $T = 0$ as in [2]).

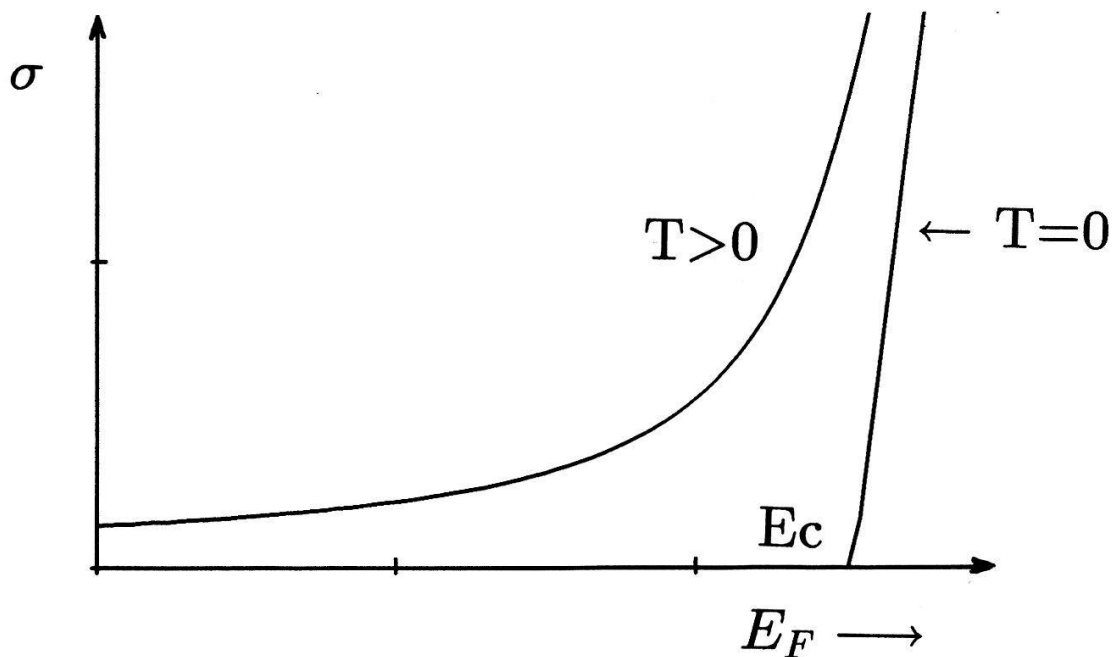


Figure 1 (see text)

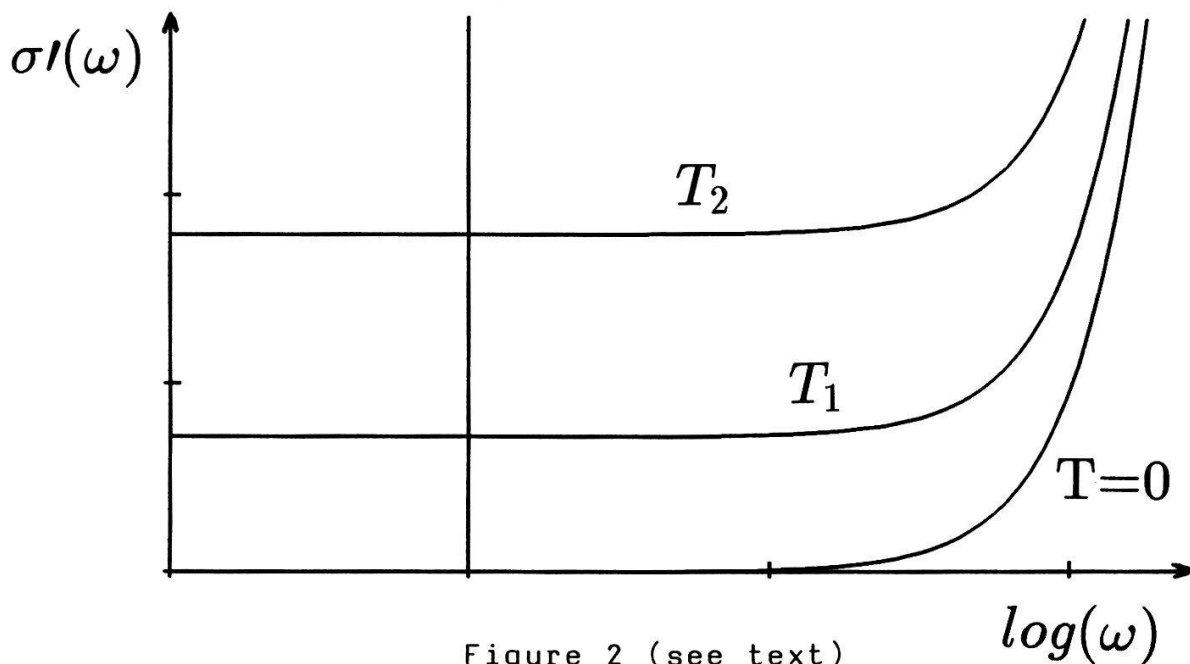


Figure 2 (see text)

The frequency dependence of $\sigma'(T, \omega)$ is shown in Fig. 2 for different temperatures, ($T_2 > T_1 > 0$). While the frequency dependence of σ is in qualitative agreement with measurements on amorphous semiconductors [5], the observed scaling behavior of $\sigma(T, \omega)$ [5] is not given correctly. It is therefore important to investigate to what extent the theoretical approach of refs. [1], [2] used here is able to describe the mechanism of phonon induced hopping which seems to be the important aspect of transport near and below E_c [5]. Work with "energy resolved" Wigner functions (which can exhibit the energy jumps of the electrons due to phonon absorption and emission) is currently in progress.

The authors thank W. Götze, A. Shah and S. Nettel for helpful discussions. This work has been supported by the Swiss National Science Foundation.

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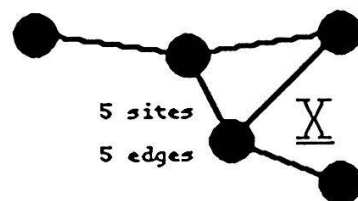
BETHE LATTICES AND INVERSE ORBITS

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Abstract: For spin systems on Bethe lattices, it will be told how the DLR (= Dobrushin-Lanford-Ruelle) problem can be solved by finding the solutions of another problem. This other problem is to find "inverse orbits" of a certain dynamical system. Some simple "inverse orbits" will be presented.

1. Brief statement of the DLR problem

Here, a spin system on the graph X (i.e. a countable set of sites with a countable set of edges) will be the set $\underline{S}^X$ of all configurations $X \rightarrow \underline{S}$, $\underline{S}$ being a finite set of "spin states". A Markov field (MF) is a probability on $\underline{S}^X$ such that, roughly: for each site x , the conditional probab. "at x ", "given the rest", depends only on the config. on the neighbors of x .



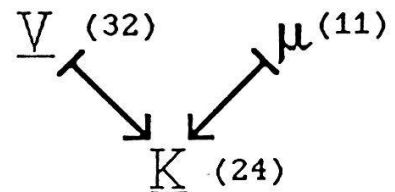
A specification (SP) is a family $K = \{K_x\}$, indexed by X , whose member K_x is a transition probab. from the config.'s on the set of the neighbors of x to the "spin states at x ". A first version of the DLR problem is: Given a SP K , find all MF's μ "having" precisely K as "their" family of transition probab.'s.

But, for a given $\underline{S}^X$, the manifold of SP's has a higher dimension than the manifold of MF's; thus, for X as in the sketch, and if $\underline{S}$ has 2 elements, $\dim\{\text{SP's}\} = 24$, $> \dim\{\text{MF's}\} = 11$. The map $\mu \mapsto K$ being smooth, K has to satisfy restrictions if K must "come from" some μ . This question of compatibility has an answer with a physical ring: K "comes from" some μ iff K "comes from" some neighbor potential (NP) V , through a "Boltzmann-like" prescription: roughly, $K_x \sim e^{-\sum V}$; see [1], Sect.2.3 for details.

A NP V is a family of real valued "potentials" V , one for

each clique of neighboring sites. A second version of the DLR problem is then: Given a NP $\underline{V}$, find all MF's μ such that the SP $\underline{K}$ "coming from" $\underline{V}$ is precisely the SP "coming from" μ . The set of all these MF's is often denoted by $\underline{G}(\underline{V})$, 'G' as in 'Gibbs'.

If $\underline{X}$ is finite, then $\underline{G}(\underline{V})$ has always exactly 1 element, for any $\underline{V}$. On the other hand, if $\underline{X}$ is infinite, there are cases where $\underline{G}(\underline{V})$, which always has at least 1 element, has actually more than 1 element. This mathematical phenomenon is commonly thought to be a simile for the physical phenomenon of phase transition. The present work is about some of the simplest cases of such a phenomenon.

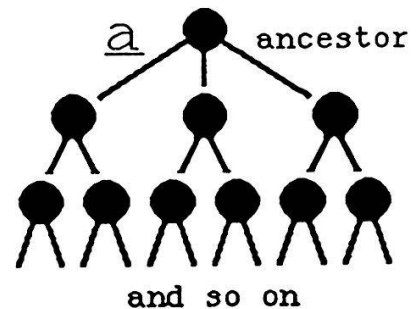


the numbers give the dimensions, for $\underline{X}$ and $\underline{g}$ as in the text

2. Spitzer NP's, Bethe maps and inverse orbits

Such simple cases occur on the graphs called Bethe lattices.

A Bethe lattice (BL) is a graph with the special properties: i) that it is a "tree" (no loops); and ii) that each site has the same number $N+1$ of neighbors (up to graph isomorphisms, N gives a unique BL). We shall pick out a site $\underline{a}$ as ancestor, thus defining a unique father-son relation between sites.

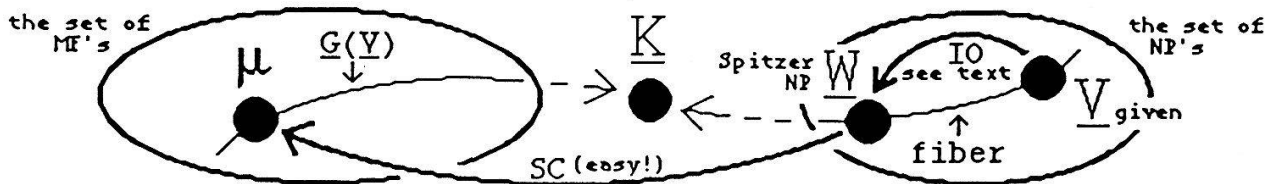


and so on

case $N = 2$

On a BL with ancestor $\underline{a}$, there is a useful special kind of NP's, which we call Spitzer NP's, in homage to [2]. Def.: a NP $\underline{V}$ is a Spitzer NP iff there is: i) $\pi: \underline{S} \rightarrow \mathbb{R}$ with $\pi(s) > 0$ and $\sum_s \pi(s) = 1$, and ii) $M_{\underline{z}}: \underline{S} \times \underline{S} \rightarrow \mathbb{R}$ with $M_{\underline{z}}(r, s) > 0$ and $\sum_s M_{\underline{z}}(r, s) = 1$ (for each site $\underline{z} \neq \underline{a}$); such that: a) $V_{\{\underline{z}\}} = 0$ if $\underline{z} \neq \underline{a}$, b) $\exp(-V_{\{\underline{a}\}}(\omega)) = \pi(\omega(\underline{a}))$, c) $\exp(-V_{\{\underline{z}, \underline{y}\}}(\omega)) = M_{\underline{z}}(\omega(\underline{z}), \omega(\underline{y}))$ (when $\underline{y}$ is the "son" of $\underline{z}$). The nice feature is this: if $\underline{V}$ is a Spitzer NP, it is **easy** to construct a MF μ belonging to $\underline{G}(\underline{V})$ ([2], p.388; see [1], Sect. 3.2).

The idea is now to use this "Spitzer construction" (SC) to solve the DLR problem in its 2nd version. Let $\underline{V}$ be a NP with SP $\underline{K}$; to find a MF μ belonging to $\underline{G}(\underline{V})$, first find a Spitzer NP $\underline{W}$ "in the fiber of $\underline{V}$ ", i.e. with the same SP, then apply SC to $\underline{W}$:



For the case of a homogeneous NP $\underline{V}$ - $\underline{V}$ is homogeneous iff there is $G: \underline{S} \times \underline{S} \rightarrow \mathbf{R}_{>}$, symm., and $H: \underline{S} \rightarrow \mathbf{R}_{>}$ such that $V_{\{\underline{z}\}}(\omega) = H(\omega(\underline{z}))$ (all sites) and $V_{\{\underline{z}, \underline{y}\}}(\omega) = G(\omega(\underline{z}), \omega(\underline{y}))$ (all pairs of neighbors) - define the Bethe map $B: \mathbf{R}_{>}^{\underline{S}} \times \dots \times \mathbf{R}_{>}^{\underline{S}}$ (N times) $\rightarrow \mathbf{R}_{>}^{\underline{S}}$ by

$$B(c_1, \dots, c_N)(r) = (\sum_s G(r, s) H(s) c_1(s)) \dots (\sum_s G(r, s) H(s) c_N(s)).$$

An inverse orbit (IO) for $\underline{V}$ is a family $c = \{c_{\underline{x}}\}_{\underline{x} \in \underline{X} \setminus \{\underline{a}\}}$ such that $c_{\underline{x}} = B(c_1, \dots, c_N)$ ($\{1, \dots, N\}$: the set of the sons of $\underline{x}$).

Now, it turns out that any IO for the homogeneous NP $\underline{V}$ **easily** gives a Spitzer NP $\underline{W}$ "in the fiber of $\underline{V}$ ". Then, by SC, we **easily** get from $\underline{W}$ a MF μ belonging to $\underline{G}(\underline{V})$.

This is the sense in which the DLR problem is replaced by the IO problem. See [1] for details.

3. An example: the diagonal case

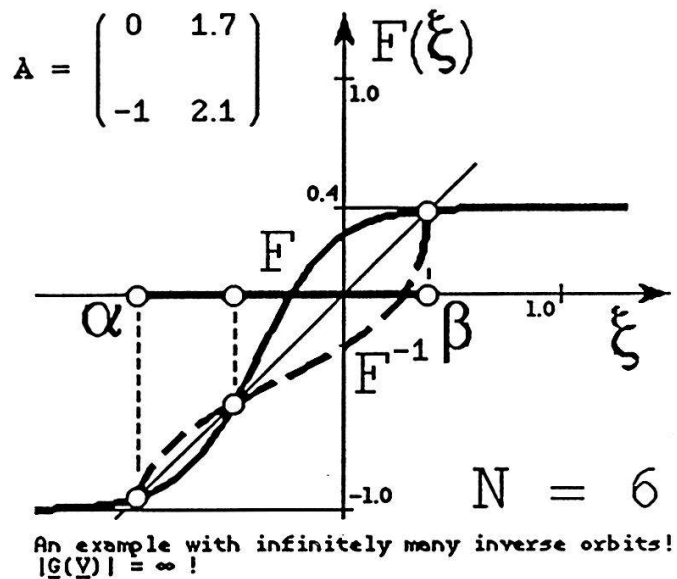
If, starting from a homogeneous NP $\underline{V}$ given by G and H , as above, we ask for those Spitzer NP's in the fiber of $\underline{V}$ which are invariant with respect to all those graph isomorphisms which leave the ancestor $\underline{a}$ invariant, we must look for those IO's c such that $c_{\underline{x}}$ depends only on the distance n between $\underline{a}$ and $\underline{x}$: there is a $\mathbf{R}_{>}^{\underline{S}}$ -valued map b defined on the positive integers such that $c_{\underline{x}} = b(n)$. Obviously, c is an IO iff b is itself an inverse orbit in the sense that $b(n) = B_d(b(n+1))$, where the diagonal Bethe map $B_d: \mathbf{R}_{>}^{\underline{S}} \rightarrow \mathbf{R}_{>}^{\underline{S}}$ is given in terms of B by $v = B_d(u) = B(u, \dots, u)$ (N times 'u') for any $u \in \mathbf{R}_{>}^{\underline{S}}$.

When $\underline{S}$ has only 2 elements, one can see that: to find an IO for B_d is equivalent to find an IO of a map $F: \mathbf{R} \rightarrow \mathbf{R}$ of the form

$$F(\xi) = \log \frac{\exp(A_{21}) + \exp(A_{22} + N\xi)}{\exp(A_{11}) + \exp(A_{12} + N\xi)};$$

G and H give the matrix A ; this map $(G,H) \mapsto A$ turns out to be surjective onto the set of all 2×2 real matrices.

The figure shows an example where F has infinitely many IO's: $\underline{G}(\underline{V})$ contains an infinite number of MF's! Restricted to the closed interval between the fixed points α and β , F here is a bijection with inverse F^{-1} . Any "direct" orbit $\{\xi_n\}$ of F^{-1} (ξ_0 arbitrary in $[\alpha, \beta]$, $\xi_{n+1} = F^{-1}(\xi_n)$) is an inverse orbit of F : $\xi_n = F(\xi_{n+1})$!



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Dépendance en température de la résistivité électrique dans le système $\text{YBa}_2\text{Cu}_3\text{O}_{7.8}$ sous l'action d'un champ magnétique

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Résumé

La résistivité a.c. de deux barreaux de $\text{YBa}_2\text{Cu}_3\text{O}_{7.8}$ a été étudiée en fonction de la température sous l'action d'un champ magnétique longitudinal. Les résultats expérimentaux montrent que l'effet du champ magnétique sur la résistivité devient prépondérant seulement pour $T < T_s$, où T_s a pu être déterminée à l'intérieur de la région de transition.

Introduction

La découverte des pérovskites supraconductrices à haute T_c [1], [2] a ouvert la voie à d'intéressantes perspectives dans des domaines aussi variés que la recherche de nouveaux matériaux à haute T_c [3], les films supraconducteurs [4] avec l'électronique basée sur l'effet Josephson, sans oublier le formidable défi théorique qu'il faut relever pour arriver à une compréhension cohérente de ce nouveau phénomène.

Notre but dans ce travail a été d'étudier dans quelques échantillons de structure $\text{YBa}_2\text{Cu}_3\text{O}_{7.8}$ leur résistivité a.c. en fonction de la température sous l'action d'un champ magnétique. Au cours de l'expérience, la direction du champ magnétique était parallèle à l'axe principal de l'échantillon et au courant a.c. circulant dans celui-ci, son intensité ne dépassant pas quelques dizaines de gauss. Nous présentons quelques résultats préliminaires obtenus dans la région proche de la température de transition.

Préparation des échantillons et système de mesure

Les échantillons de $\text{YBa}_2\text{Cu}_3\text{O}_{7.8}$ ont été préparés par frittage suivant les procédés habituels utilisés pour ces composés. Le pressage des échantillons s'est fait en exerçant des pressions différentes : 4 tonnes/cm² pour le premier et 3 tonnes/cm² pour le second. Des moules spéciaux nous ont permis de donner à ces échantillons la forme particulière de barreaux à section rectangulaire avec des dimensions typiques de quelques mm. Ainsi, pour le premier échantillon, les dimensions étaient : longueur = 11.4 mm, largeur = 3.3 mm et hauteur = 1.6 mm. A la température $T=296$ K, les résistivités mesurées en a.c. étaient de $\rho=15.45 \mu\Omega\text{m}$ pour le premier échantillon et de $\rho=13.43 \mu\Omega\text{m}$ pour le second. Ces résistivités a.c. ont

été mesurées à la fréquence de 300 Hz au moyen d'un amplificateur "lock-in" et en utilisant un système de mesures à 4 points. Nous avons opéré avec la même fréquence dans le domaine de température s'étendant depuis la température ambiante jusqu'à la température de transition. La densité de courant j existant dans l'échantillon était comprise dans les limites $4.76 \times 10^{-2} \text{ A/cm}^2 < j < 6.67 \times 10^{-2} \text{ A/cm}^2$ et la mesure de la température s'est faite avec un thermomètre de platine.

Résultats expérimentaux et discussion

Les Figs. 1 et 2 montrent les courbes $\rho = \rho(T, H)$ pour les deux échantillons de $\text{YBa}_2\text{Cu}_3\text{O}_{7.8}$ mesurés. Elles ont été obtenues en appliquant d'abord le champ magnétique H sur l'échantillon qui se trouvait initialement à la température ambiante, et en le refroidissant ensuite lentement jusqu'à la température de transition. Le commencement de la transition supraconductrice est à $T \approx 97 \text{ K}$ pour le premier échantillon et à $T \approx 95 \text{ K}$ pour le second.

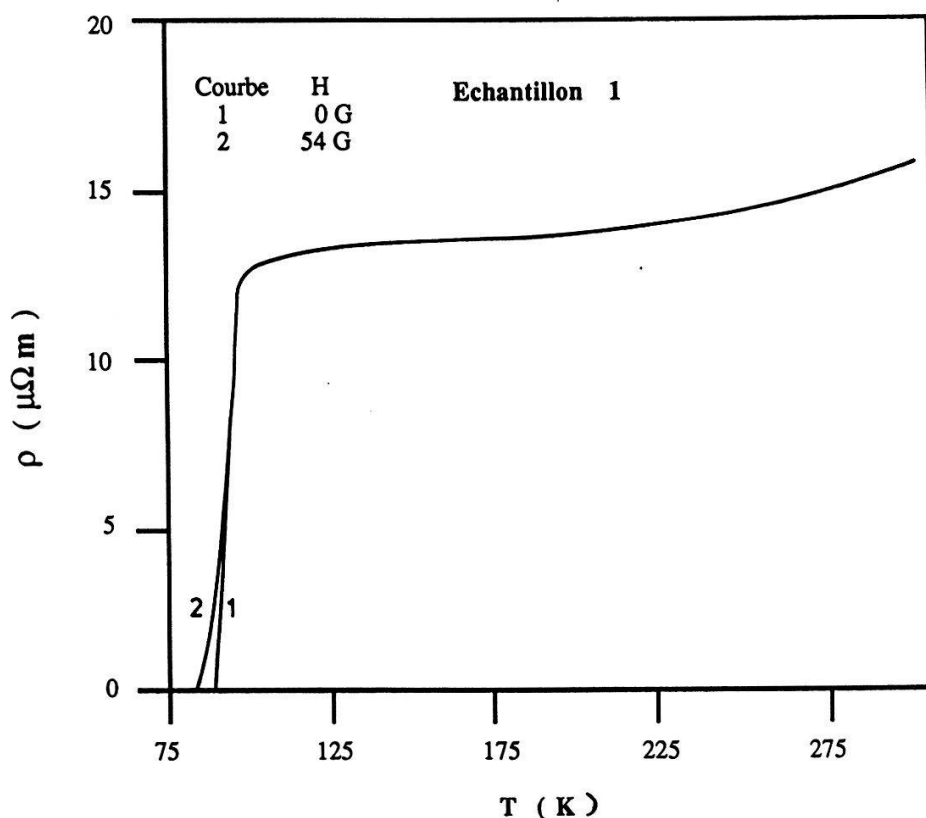


Fig.1. Comportement des courbes $\rho = \rho(T, H)$ dans le domaine de température allant depuis la température ambiante jusqu'à celle de transition. Une différence notable apparaît entre ces deux courbes à partir de $T < T_s \approx 93 \text{ K}$ où $\rho(T; H=54 \text{ G}) > \rho(T; H=0)$.

Dans la Fig.1 qui correspond au premier échantillon, on peut voir pour l'ensemble de ce domaine de température l'effet que produit sur ρ un champ magnétique d'intensité $H=54$ G. Les résultats indiquent notamment que pour des températures telles que $T > T_s$, où $T_s \approx 93$ K se situe dans la région de transition, la magnétorésistance est pratiquement négligeable et $\rho(T; H=54 \text{ G}) \approx \rho(T; H=0)$. Par contre, lorsque $T < T_s$, les deux courbes se séparent et l'on constate alors que $\rho(T; H=54 \text{ G}) > \rho(T; H=0)$.

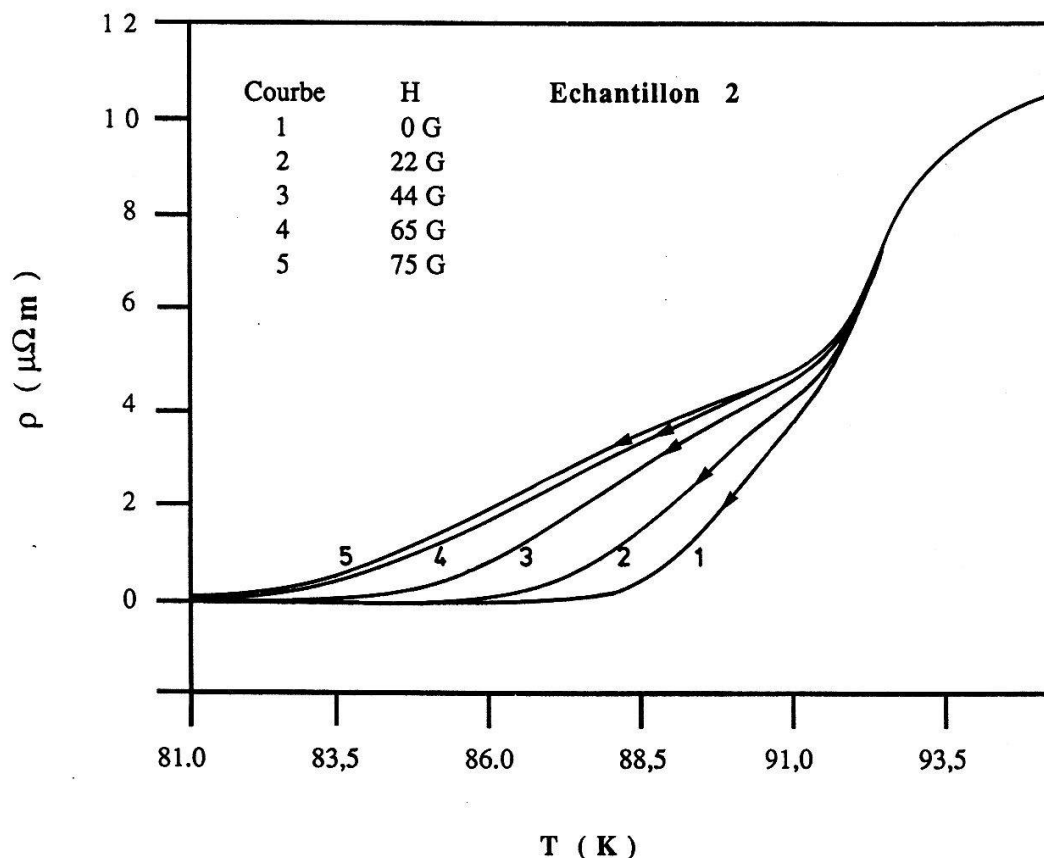


Fig.2. Etude des courbes $\rho = \rho(T, H)$ dans la région de transition pour plusieurs valeurs du champ magnétique. Lorsque $T < T_s \approx 92.5$ K, les résistivités obéissent à la relation $\rho(T, H_2) > \rho(T, H_1)$ pour $H_2 > H_1$. On peut voir que $\rho \sim T$ dans une partie importante de ce domaine.

Ce comportement général est corroboré par l'étude réalisée sur le deuxième échantillon. La Fig. 2 montre plus en détail la région d'intérêt où l'on peut observer que les courbes s'échelonnent suivant la relation $\rho(T, H_2) > \rho(T, H_1)$ lorsque $H_2 > H_1$ et $T < T_s \approx 92.5$ K. A première vue, ces données expérimentales peuvent s'expliquer par le fait que, lorsque $H \neq 0$, le supraconducteur doit expulser le champ magnétique. Pour cette raison, il faut s'attendre à mesurer une plus grande résistivité ainsi qu'une température de transition plus basse. Dans cette région, le supraconducteur serait dans une phase métastable pouvant être décrite par le modèle de "verre de spin" d'Almeida et Thouless [5], [6]. Pour ces valeurs du champ magnétique et à

partir de T_s , la variation initiale de ρ en fonction de T est pratiquement linéaire avec une pente proportionnelle à $1/H$. Ensuite cette tendance disparaît et ρ décroît de manière presque asymptotique jusqu'à l'expulsion complète du champ magnétique avant de s'annuler.

Conclusions

Ce travail nous a montré qu'en présence d'un champ magnétique et en-dessous d'une certaine température T_s (inférieure à la température marquant le début de la transition), les courbes donnant la résistivité des échantillons de $\text{YBa}_2\text{Cu}_3\text{O}_{7.8}$ se séparent et obéissent à la relation $\rho(T, H_2) > \rho(T, H_1)$ lorsque $H_2 > H_1$. Nous avons aussi constaté que dans un large domaine de cette région, ρ variait linéairement avec T , la pente étant proportionnelle à $1/H$. Il est à remarquer que la courbe de résistivité pour laquelle $H=0$ présente également cette variation linéaire en T .

Les auteurs remercient le Fonds National Suisse pour la Recherche Scientifique pour son soutien financier, J. Rittener et R. Schöpfer pour leur aide technique.

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