Zeitschrift: Helvetica Physica Acta
Band: 56 (1983)
Heft: 1-3

Artikel: Positrons and solid state physics
Autor: Manuel, A.A.
DOI: https://doi.org/10.5169/seals-115389

Helvetica Physica Acta,
Vol. 56 (1983) 437-448

0018-0238/83/010437-12$1.50+0.20/0

POSITRONS AND SOLID STATE PHYSICS

A.A. MANUEL

Department of Physics, University of Geneva
Bd d'Yvoy 32, CH-1211 Geneva 4, Switzerland

INTRODUCTION

Positron annihilation (PA) is used for many purposes in solid state physics. We outline the principles of this method in section 1. In sections 2 to 5 we illustrate how positrons are used to study problems as different as particle diffusion through a solid, defects in crystals and amorphous materials, electron momentum distributions, Fermi surface measurements or surfaces states. The reader is refered to complete review papers [1-3] and conference proceedings [4,5] for more detailed discussions.

1. POSITRON ANNIHILATION

Positrons used are usually emitted by radioactive sources (^{22}Na, ^{58}Co, ^{64}Cu) with a maximum kinetic energy of about 0.5 MeV. When they penetrate a solid they thermalize much quicker (1 psec.) than their mean lifetime (100 psec. in pure metals). After diffusion, they finally annihilate with an electron of the solid. In the most frequent annihilation process, two γ-rays are emitted which are detected to yield information about the annihilated electron-positron (e-p) pair. Two properties of the annihilation process are usually measured independently : the lifetime of the positron and the e-p pair momentum.

1.1 Positron lifetime

The lifetime of the positron depends mainly on the electron density around the positron. Therefore PA is suitable to investigate charge transfer, positron dynamics, e-p correlations and defects. The lifetime is determined by recording the time elapsed between the detection of the "positron birth marker", a γ-ray emitted with the positron during the β-decay, and the annihilation radiation. Currently, lifetime spectrometers have a

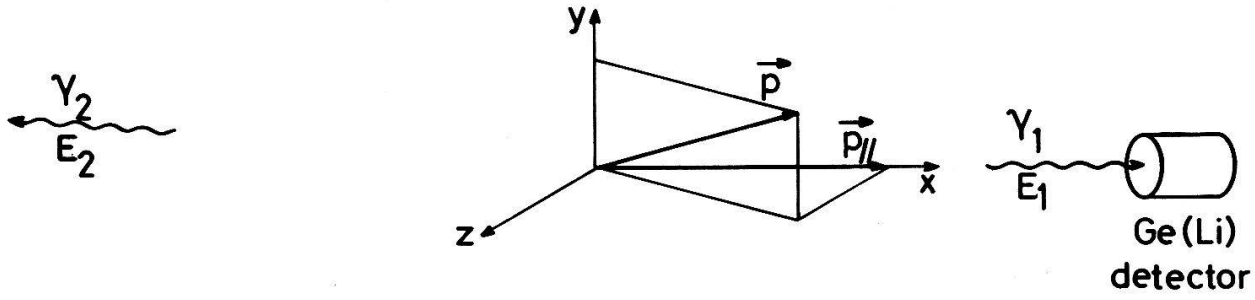
time resolution of 280 psec. [6].

1.2 The electron-positron pair momentum

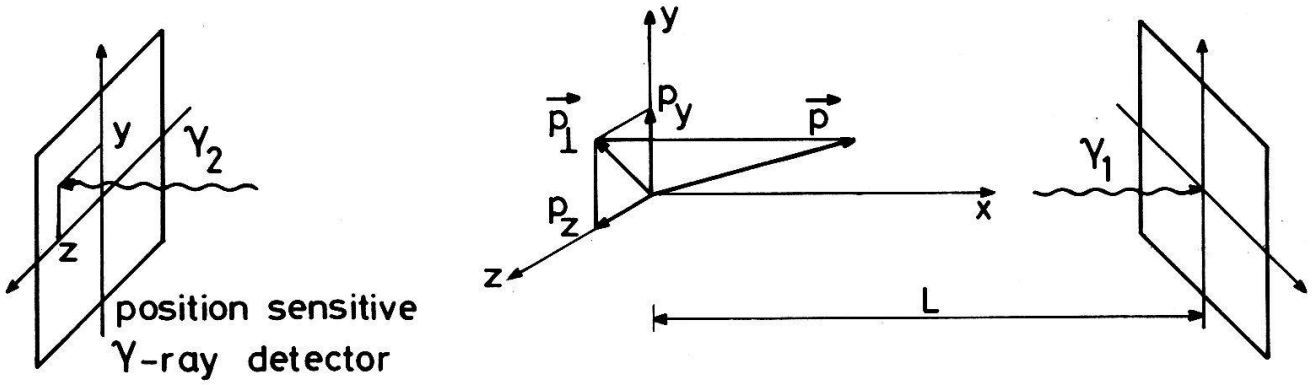
By momentum conservation, the annihilation radiation carries the momentum of the annihilated e-p pair. There are two different ways to measure this pair momentum :

a) Doppler broadening of the annihilation line :

If the annihilated pair is at rest, each of the two γ-rays has an energy of E_o=511 KeV which is just the mass energy of the annihilated particles. A shift of few KeV is induced by Doppler effect if the pair is not at rest. This shift is proportional to the pair momentum $\vec{p}_{//}$ along the direction of the γ-rays, as schematically shown in Fig. 1.a. It is given by :



a. Doppler broadening



b. Angular Correlation

Fig. 1 Geometries used for PA measurements :
a) Doppler broadening, b) 2D-ACPAR.

$$|\vec{P}_{//}| = \frac{2}{c}(E_1 - E_o) \qquad (1)$$

The Doppler broadening technique is characterized by a high counting rate but its resolution is limited by available detectors.

b) Angular correlation of the PA radiation (ACPAR) :

The two annihilation γ-rays are emitted in nearly opposite directions. A deviation of some milliradians from the straight line is proportional to the momentum $\vec{p}_\perp$ perpendicular to the direction of the γ-rays. The ACPAR technique is characterized by a good resolution of the momentum (0.03 a.u.) but its counting rate may be three orders of magnitude below the Doppler broadening technique.

Recently, the possibilities offered by ACPAR measurements have been increased considerably by the use of bidimensional position sensitive γ-ray detectors [7-9]. If $\rho^{2\gamma}(\vec{p})$ is the momentum distribution of the annihilation radiation, these 2D-ACPAR machines produce a 2D-distributions $N(p_y,p_z)$ which is given by :

$$N(p_y,p_z) = \int_{-\infty}^{+\infty} \rho^{2\gamma}(\vec{p})\, dp_x \qquad (2)$$

where x is the direction of the propagation of the γ-rays, as shown in Fig. 1.b.

2. DYNAMICS OF POSITRONS IN SOLIDS

To know how positrons move in the solid is essential for interpreting PA. Implantation profiles [10] tell us about the thermalization processes and diffusion constants [11]. These processes may be largely influenced by the internal structure of the solid. For example, it has been shown that positrons are very sensitive to the inhomogeneous charge distribution encountered in graphite intercalation compounds (GIC) [12]. As shown in Fig. 2, the ACPAR curves are very similar to pure graphite for stage n=5 intercalated donor compounds where positrons are forced, by the Coulomb repulsion, to sample the carbon layers.

In metals, the positron is screened by the conduction

electrons and its effective mass may be deduced from ACPAR measurements [13]. Electron-positron as well as electron-electron

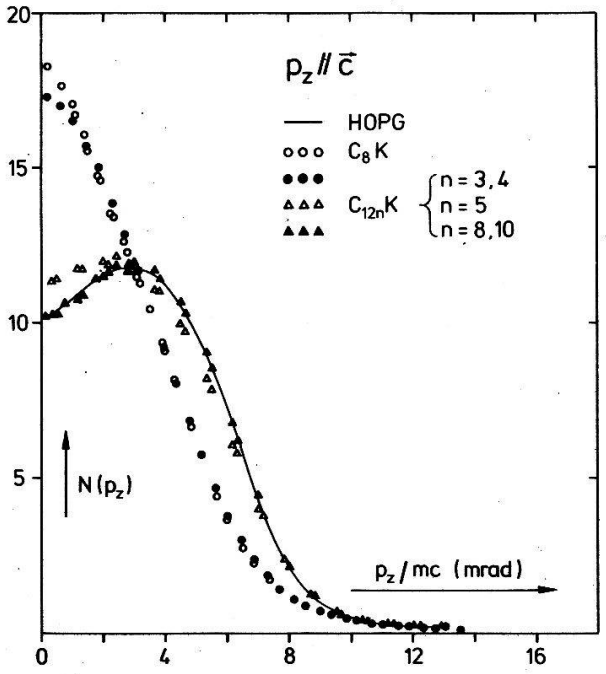


Fig. 2
ACPAR curves of highly oriented pyrolytic graphite (HOPG) and potassium intercalated graphite at different stages (From Ref. 12)

correlations may also be studied by the ACPAR technique. They manifest themselves by "enhancement" effects which were first calculated by Kahana [14]. A considerable work has been done to go beyond the approximations used in this early calculation [15,16]. In low electron density solids, it is possible to observe e-p bound states called "quasi-positronium". Their study gives a precise understanding of dynamics of e-p pairs in solids [17].

3. CRYSTAL DEFECTS AND AMORPHOUS METALS

The study of defects in materials is probably the largest field of application for PA. It was found early that during their diffusion, positrons are very sensitive to vacancies, voids, dislocations etc. Positrons are strongly repelled by ions so their density distribution is large in the interstitial region. If a positron moves near a vacancy, it can get trapped [18,19] with longer lifetimes than in the perfect lattice, because the electron density is lower. The localization of positrons at a vacancy site is shown in Fig. 3 where the positron wave function has been calculated [20] around an iron vacancy

and a carbon-vacancy pair. The result of such calculations is used to interpret positron lifetime measurements [21] which may be characterized by two or three differents components.

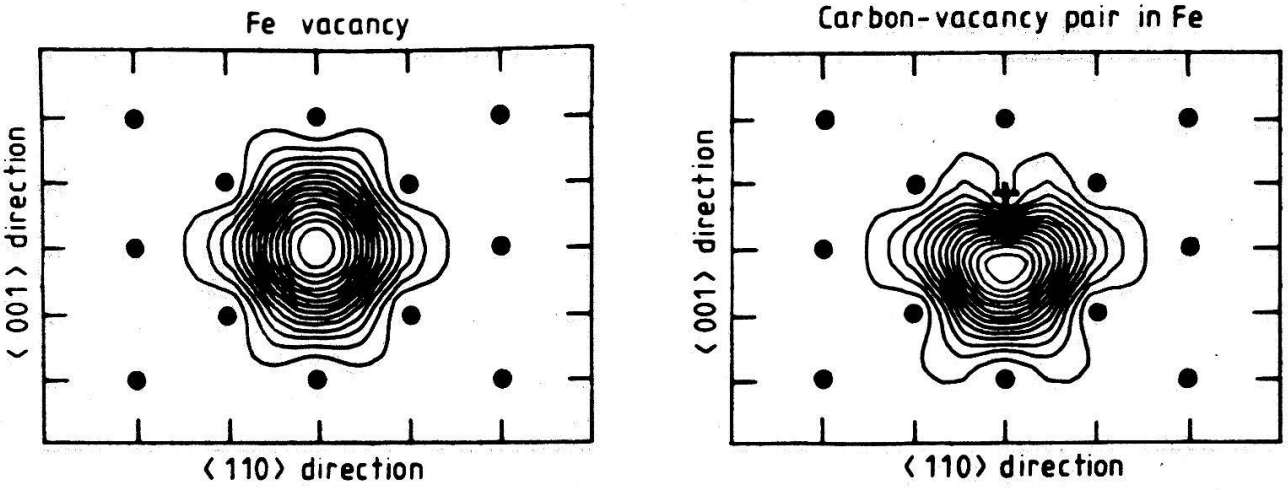


Fig. 3 The wave function of a positron trapped in a Fe vacancy and a carbon-vacancy pair in Fe. Dots are Fe atoms and the cross is the carbon atom. (From Ref. 20, with the permission of the Institute of Physics).

To measure how the intensity of these components change with temperature, irradiation, aging etc. is a very developed technique in metallurgy [22-24].

Momentum parameters (Doppler and ACPAR) are also very sensitive to defects. Recently, ACPAR distributions have been calculated and measured in quenched and annealed Al [25] as well as in Al with thermally induced vacancies [26]. Both studies take major changes in the structures into account and the behaviour is well understood as a result of defects.

PA is also used to study the nature of disorder in amorphous metals [27,28]. It has been found that, in "as received" samples, the lifetime has an intermediate value between pure metals and metals with vacancies [29]. This result is interpreted either as "small vacancies" (having 0.6 of the volume of a vacancy in the crystalline state) or as a "dislocation dipole like" [30]. In addition, it has been shown that electron

irradiation of amorphous metals produces metastable vacancies which recover continuously between 77K and 300K so that no radiation induced vacancy-like defects remain above room temperature [29].

4. ELECTRON MOMENTUM DISTRIBUTION (EMD) AND FERMI SURFACE (FS)

The ACPAR technique is very well suited to study EMD and FS. In the independant particle approximation, the two photons momentum density $\rho^{2\gamma}(\vec{p})$ (PMD) is given by :

$$\rho^{2\gamma}(\vec{p}) = \varepsilon(\vec{p}) \cdot \sum_{\substack{\vec{k} \\ n, k_{occ}}} \left| \int e^{-i\vec{p}\vec{r}} \psi_{\vec{nk}}(\vec{r}) \psi_{+}(\vec{r}) d^3r \right|^2 \qquad (3)$$

where $\psi_{\vec{nk}}(\vec{r})$ and $\psi_{+}(\vec{r})$ are the electron and positron wave functions. This quantity is equal to the EMD if $\varepsilon(\vec{p})$=cte and $\psi_{+}(\vec{r})$=1. These conditions are not fare to be true and then, according to Equ. 2, ACPAR measurements give planar projections of the EMD which may be used to build the full EMD [31-34]. By using the periodicity of the reciprocal lattice vector, it is furthermore possible to reduce the projections into the first Brillouin zone and it can be shown [34-36] that the reduced distribution has the following properties :

- the contribution of the filled bands is a constant,
- the contribution of partially filled bands is only determined by the occupation numbers $n(\vec{k})$=1 if $|\vec{k}| < k_F$.

Such reduced distributions are planar (2D-)'projections of the FS and it is possible to reconstruct the 3D-FS from such 2D-projections [37].

The ACPAR method has been applied with success to many metals and alloys since the pioneering work of Berko and Plaskett [38]. A careful comparison of the measured PMD and those calculated using Equ. 3 gives precise information about the correlation effects [34,39,40] such as the enhancements effects mentioned in section 2. For example, in pure metals, ACPAR has permitted to study the FS of bcc Li [41,42] at a temperature above the martensitic transformation. The non sphericity of this FS is measured

precisely and can be tested against non-local many body potential FS calculations [43]. It is also possible to take advantage of the polarization of positrons emitted by β-decay to study the FS of the two spin directions in magnetized metals [44-46].

Beyond pure metals, ACPAR is very powerful to investigate electronic structures of alloys and intermetallic compounds. It has the advantage to be not sensitive to a reduced mean free path, as opposed to methods based on the cyclotronic resonance. For example, PA has been successfully used to measure the change of the FS topology in Cu- and Aℓ-based non dilute alloys [34,47] and of Nb-Mo alloys [42,48,49]. Complete reconstruction of the FS has been performed in the high temperature superconducting compound V_3Si [34,37] the measured and calculated FS are in good agreement as can be seen on Fig. 4.

5. SLOW POSITRONS AND SURFACES

The latest development in PA is the production of beams of slow positrons (SP) having eV to KeV kinetic energy [50]. The SP are obtained by moderating positrons from radioactive sources. Using high density materials with negative positron work function, positrons may diffuse to the surface and be re-emitted before annihilation. These SP are focalized on samples by conventional beam techniques. The actual yield of SP is about 10^{-3} and many groups are working to increase it as well as the brightness and to reduce the energy dispersion of the SP beams.

The study of a large number of new processes is made available with SP beams. They are all related to the fact that positrons do not penetrate deeply in solids but stay near the surface or may be bound in their image potential at the surface. SP may be used to investigate defect structures below the surface [51] but they can also be re-emitted as SP, as surface positronium [52-54] in its ground state or excited states or as positronium negative ion [55].

A very promising application for SP beams is the study of surfaces directly. Although this field is just starting to

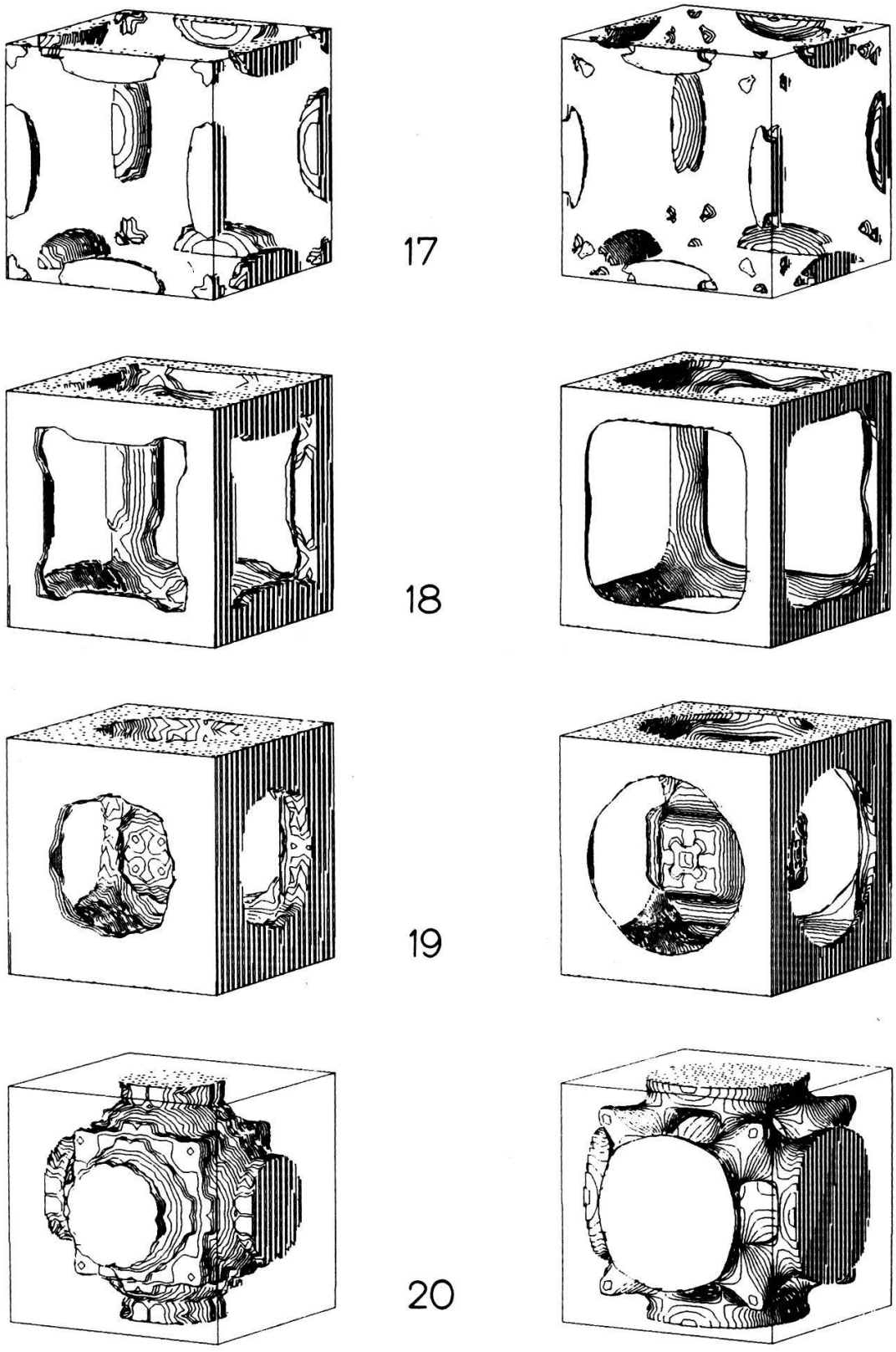


Fig. 4 The measured (left) and calculated (right) FS of V_3Si. Hole (electron) sheets are drawn for bands 17-19 (20) respectively. (From Ref. 37).

develop, one can expect progress in the near future. For example, Low Energy Positron Diffraction (LEPD) [56] is an interesting alternative to its electron counterpart (LEED). The advantages are an increased surface sensitivity (shorter elastic mean free path), and simplified calculations of the diffractions due to the absence of spin exchange and reduction of correlation with core electrons.

6. CONCLUSION

This brief overview has shown the many (and steady increasing) aspects of use of positrons for various purposes in solid state physics. We have been rather short and illustrated our presentation with some examples, not forget that much more remains. Thus, we have mainly focused our attention to metals and have not paid enough attention to the ionic crystals, polymers, semiconductors, etc. We hope that the references included will be useful to complete this overview.

Acknowledgments

I thank S. Berko, C. Corbel, P. Descouts, A. Dupasquier, K. Fujiwara, M. Hasegawa, F. Heinrich, T. Jarlborg, P. Mijnarends, A.P. Mills, P. Moser, F.M. Mueller, R.M. Nieminen, R. Paulin, L. Pecora, M. Peter, R.M. Singru, A.T. Stewart, H. Stachowiak and S. Wakoh for making available their recent results and for valuable comments on the actual trends in their speciality. I dedicate this overview to Prof. W. Brandt, a pioneer in this field, who left us early in 1983. I am grateful to the organising committee of the EPS-CMD3 conference for giving me the opportunity to present this review.

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