

Zeitschrift: Helvetica Physica Acta

Band: 62 (1989)

Heft: 6-7

Artikel: Local structure of the chemisorption of Co on Si(111)7x7 and of the epitaxial CoSi₂ interface

Autor: Rossi, G. / Santaniello, A. / Fadova, P. de

DOI: <https://doi.org/10.5169/seals-116059>

Nutzungsbedingungen

Die ETH-Bibliothek ist die Anbieterin der digitalisierten Zeitschriften auf E-Periodica. Sie besitzt keine Urheberrechte an den Zeitschriften und ist nicht verantwortlich für deren Inhalte. Die Rechte liegen in der Regel bei den Herausgebern beziehungsweise den externen Rechteinhabern. Das Veröffentlichen von Bildern in Print- und Online-Publikationen sowie auf Social Media-Kanälen oder Webseiten ist nur mit vorheriger Genehmigung der Rechteinhaber erlaubt. [Mehr erfahren](#)

Conditions d'utilisation

L'ETH Library est le fournisseur des revues numérisées. Elle ne détient aucun droit d'auteur sur les revues et n'est pas responsable de leur contenu. En règle générale, les droits sont détenus par les éditeurs ou les détenteurs de droits externes. La reproduction d'images dans des publications imprimées ou en ligne ainsi que sur des canaux de médias sociaux ou des sites web n'est autorisée qu'avec l'accord préalable des détenteurs des droits. [En savoir plus](#)

Terms of use

The ETH Library is the provider of the digitised journals. It does not own any copyrights to the journals and is not responsible for their content. The rights usually lie with the publishers or the external rights holders. Publishing images in print and online publications, as well as on social media channels or websites, is only permitted with the prior consent of the rights holders. [Find out more](#)

Download PDF: 09.01.2026

ETH-Bibliothek Zürich, E-Periodica, <https://www.e-periodica.ch>

LOCAL STRUCTURE OF THE CHEMISORPTION OF CO ON Si(111)7x7
AND OF THE EPITAXIAL CoSi₂ INTERFACE

G. Rossi,* A. Santaniello, P. De Padova, X. Jin and D. Chandesris

Laboratoire pour L' Utilisation du Rayonnement Electromagnétique,
CNRS-CEA-MEN, Univ. Paris-Sud, F-91405 Orsay, France
*and Laboratorium fur Festkorperphysik, ETH Honggerberg, CH 8093
Zurich, Switzerland

Abstract: The atomic environment of Co atoms deposited at room temperature on the Si(111)7x7 surface, and of Co in the interface CoSi₂ epitaxial layer grown on Si(111)7x7 by thermal annealing are investigated by means of surface-extended-X-ray-absorption-fine-structure on the Co K-edge. Models for the chemisorption sites and epitaxial interfaces are directly derived from the SEXAFS results.

1. Introduction

The bonding geometry at the transition metal/semiconductor interface is a key knowledge for the understanding of the physical properties of Schottky junctions, multilayers and heterostructures. Co/Si(111)7x7 is a model system in this class since epitaxial growth of a metallic silicide, CoSi₂, is easily obtained, and both electrical and optical properties of these epitaxial interfaces are intensively investigated. We present here a summary of new results obtained by SEXAFS on 0.5 monolayers (ML) of Co deposited at room temperature (RT) onto Si(111)7x7, representing the chemisorption stage, and on the same system but after flash annealing at 630 C, representing a two-dimensional CoSi₂ epitaxial layer.[1,2]

2. Chemisorption

Details of the experiments and data analysis will be published elsewhere.[2] The sample preparation was carried out in UHV ($<1\times10^{-8}$ Pa) as well as the measure of the absorption coefficient of the Co 1s core level up to 500 eV above threshold (7707 eV). The synchrotron radiation from the DCI storage ring at LURE was energy selected by a double crystal Si(311) device.

The Co K-edge SEXAFS signal contains informations on the bond distances of neighbouring atoms, and on the coordination numbers. The polarization dependence was exploited by measuring the SEXAFS with the X-rays at normal incidence (E vector in the surface plane) and at glancing incidence (E vector almost perpendicular to the surface). In this case the polarization dependent SEXAFS coordination number is $N^* = 3 \sum_i N_i \cos^2 \alpha_i$, where N_i is the number of neighbours of the i -th neighbour shell whose bonds form the angle α_i with the E vector of the X-rays. Standard Fourier analysis[5], in the $k=3.2-10 \text{ \AA}^{-1}$ range, shows lack of atomic order beyond the first neighbour shell. The SEXAFS signal sensitive to the in-plane neighbours shows only Si neighbours at one well defined distance (see table 1). A two shell analysis was necessary for the signal sensitive to the neighbours along the vertical direction, indicating that both Si and Co first neighbours are present perpendicular to the interface. The N^* 's and interatomic distances obtained are summarised in table 1.

The summary of the experimental results on the room temperature chemisorption is:

- a) anisotropic coordination number for Co-Si at 2.31 \AA interatomic distance; (table 1)
- b) existence of Co-Co neighbours at 2.56 \AA only in the vertical [111] direction; (table 1)
- c) maintain of 7×7 periodicity in the chemisorbed surface from LEED observations.

We propose in figure 2b a model for the chemisorption of 0.5 monolayers of Co onto $\text{Si}(111)7 \times 7$ at room temperature which satisfies quantitatively all the above requirements. The model is based on a "majority" Co site in the sixfold interstitial position in between the top and second $\text{Si}(111)$ layer. The N^* data relative to 0.5 Co monolayers at room temperature (table 1) indicate that .35 ML of Co can occupy such sites. (this implies lifting of the top three atoms of the Si honeycomb by $0.8(\pm 1) \text{ \AA}$) The "minority" Co site is on top of the majority site with Co bonded with three Si atoms and the Co atom lying below. 0.15 ML of Co can be accommodated into the minority sites at the coverage of 0.5 \AA discussed here. The two positions (majority and minority sites) for Co explain all of the SEXAFS distances and the relative occupation between majority and minority Co sites accounts for the SEXAFS amplitudes.

The model derived above from the SEXAFS results closely relates the chemisorption with the substrate reconstruction. Looking to the well-supported dimer-adatom-stacking-fault model for the $\text{Si}(111)7 \times 7$ reconstruction [6] (fig 2a) and disregarding

the Si adatoms one counts 20 bulklike honeycombs per 49-atom surface unit cell, half of which are in stacking fault with the substrate, plus large circular holes at the corners and oval holes along the edges and the short diagonal. The large hollow sites cannot accommodate Co in a high coordination configuration at the measured distance of 2.31\AA . The chemisorption is therefore favoured on the bulklike sixfold interstitial sites as in the related cases of chemisorption of Ni[3] and Pt[4]. The filling of all of the sixfold interstitial sites, without destroying the surface periodicity, would leave to the extra incoming Co atoms the threefold atop sites. We stress that this model which is directly derived from the SEXAFS data implies in a direct way, and for the first time, the key role played by the 7×7 reconstruction in determining the chemisorption geometry of a silicide forming metal.

3. Epitaxy

After flash annealing at 630°C the interface we obtain the SEXAFS data summarised in the second panel of fig 1. In the interface plane the distances and N*'s are: Co-8 \pm 5 Si $2.31(\pm 0.02)\text{\AA}$ and Co-9 \pm 1Co at $3.78(\pm 0.03)\text{\AA}$. Perpendicular to the interface Co-8 \pm 5 Si at $2.35(\pm 0.03)\text{\AA}$ and no Co second neighbours. This corresponds to a two dimensional (2D) layer of CoSi_2 , buried below a layer of silicon migrated to the surface, as confirmed by Auger spectroscopy. Independent evidence of Si migration on top of epitaxial CoSi_2 layers on $\text{Si}(111)$ was obtained in previous studies.[9,13] The model of the 2D epitaxial $\text{CoSi}_2/\text{Si}(111)$ interface is given in fig 2c for the A and B orientations, and has been discussed in recent letters.[1,5]

4. Conclusions

We could determine the bond distances and coordination numbers of the first neighbours of Co in two distinct situations: chemisorption at RT onto $\text{Si}(111)7\times 7$ and epitaxial CoSi_2 interface layer. From the SEXAFS results we derive a model of chemisorption which is compatible with the 7×7 reconstruction of the substrate, and we establish the eightfold coordination of Co at the interface between CoSi_2 and $\text{Si}(111)$.

5. References

- [1] G. Rossi, X. Jin, A. Santaniello, P. DePadova, and D. Chandresris; Phys. Rev. Lett. 62, 191 (1989).
- [2] G. Rossi, A. Santaniello, and P. DePadova, to be published.
- [3] F. Comin, J.E. Rowe, and P.H. Citrin; Phys. Rev. Lett. 51, 2402 (1983).
- [4] G. Rossi, D. Chandresris, P. Roubin, and J. Lecante; Phys. Rev. B34, 7455 (1896).
- [5] D.R. Hamann, Phys. Rev. Lett. 60, 313 (1988).
- [6] K. Takanayagi, Y. Tanishiro, S. Takahashi, and M. Takaahashi, Surf. Sci. 164, 367 (1985).

	CHEMISORPTION		EPILAYER		CoSi ₂	
	Co-Si	Co-Co	Co-Si	Co-Co	Co-Si	Co-Co
N* //	6.8(.5)	0(1)		8(.5)	9(1)	8 12
d//(Å)	2.31(.02)	-	2.31(.02)	3.78(.03)	2.31	3.78
N* ⊥	3.7(.5)	2.4(.5)		8(.5)	0(1)	8 12
d⊥(Å)	2.31(.03)	2.56(.03)	2.35(.03)	-	2.31	3.78

Table 1. SEXAFS results: polarization dependent coordination numbers N^* and bond distances d for Co and its nearest neighbours. Reference crystallographic data for CoSi_2 are also given.

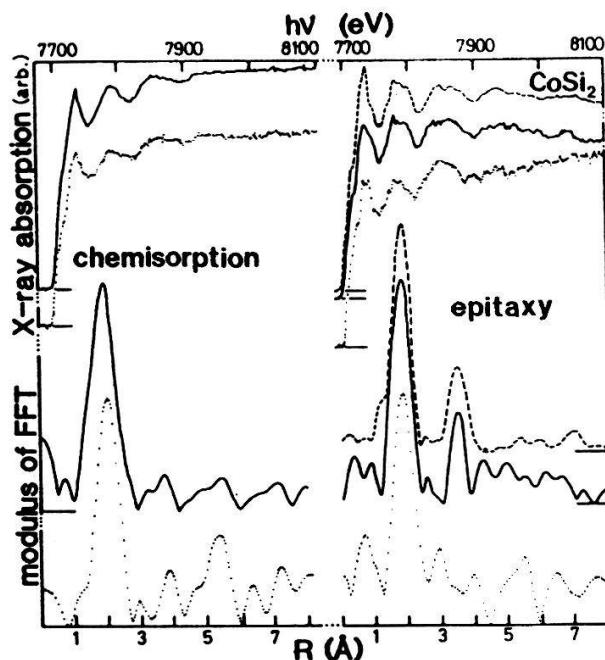


Fig. 1 Co K-edge SEXAFS spectra and modulus of Fourier transform (FFT). Left panel: chemisorption of 0.5 ML Co/Si(111)7x7. Data and FFT for normal incidence (continuous line) and grazing incidence (dotted curves). Right panel: CoSi_2 standard (dashed curves) and epitaxial 2D- CoSi_2 /Si(111) at normal incidence (continuous line) and grazing incidence (dotted curve).

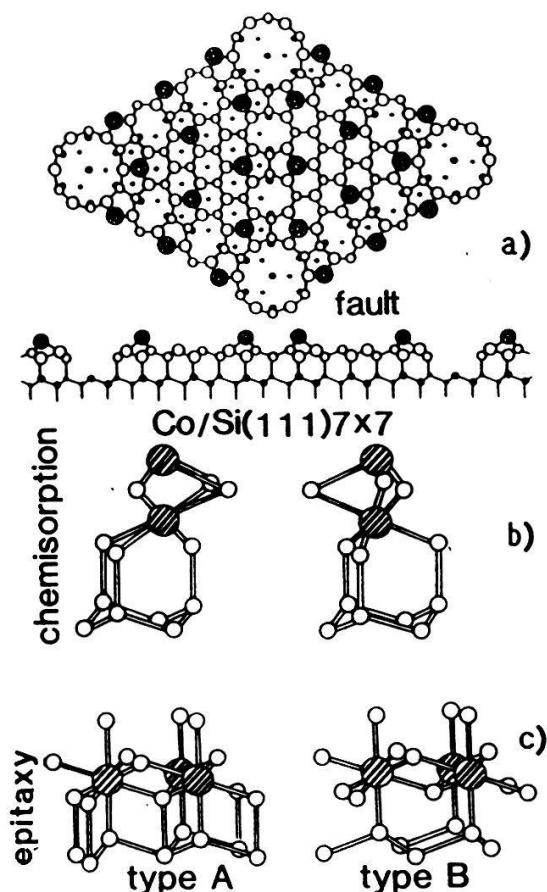


Fig.2 a) top and side view of the DAS model of Si(111)7x7. The cross hatched atoms are the Si adatoms. b) SEXAFS derived model for the chemisorption of Co (large hatched atoms) onto Si(111)7x7, both on unfaulted (left) and faulted (right) 7x7 sites. c) Hamann's models [5] of type A and B $\text{CoSi}_2/\text{Si}(111)$ interfaces compatible with the SEXAFS results on the annealed samples.