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

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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 ($<1 \times 10^{-8}$ 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 2.31Å interatomic distance;(table 1)
- b) existence of Co-Co neighbours at 2.56Å only in the vertical [111] direction;(table 1)
- c) maintain of 7x7 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 Si(111)7x7 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 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 $0.8(\pm 0.1) \text{ \AA}$) 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 0.5Å 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 Si(111)7x7 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 2.31Å. 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 7x7 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±.5 Si 2.31(±.02)Å and Co-9±1Co at 3.78(±.03)Å. Perpendicular to the interface Co-8±.5 Si at 2.35(±.03)Å and no Co second neighbours. This corresponds to a two dimensional (2D) layer of CoSi₂, buried below a layer of silicon migrated to the surface, as confirmed by Auger spectroscopy. Independent evidence of Si migration on top of epitaxial CoSi₂ layers on Si(111) was obtained in previous studies.[9,13] The model of the 2D epitaxial CoSi₂/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 Si(111)7x7 and epitaxial CoSi₂ interface layer. From the SEXAFS results we derive a model of chemisorption which is compatible with the 7x7 reconstruction of the substrate, and we establish the eightfold coordination of Co at the interface between CoSi₂ and Si(111).

5. References

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	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 CoSi₂ are also given.

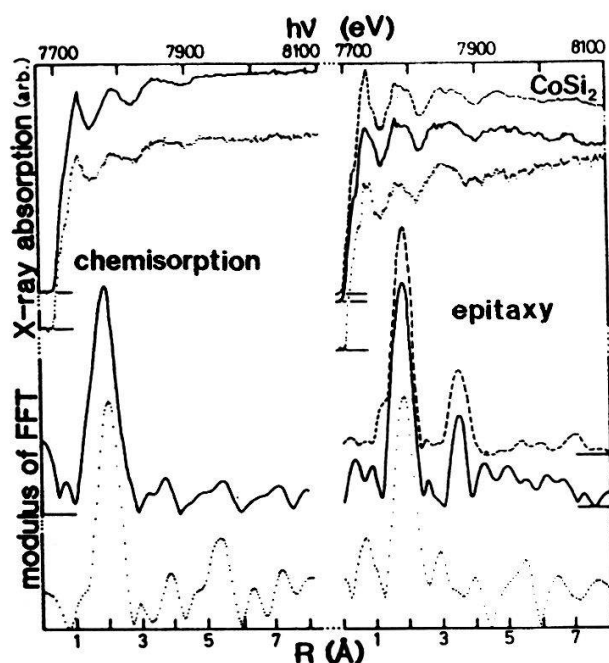


Fig.1 Co K-edge SEXAFS spectra and modulus of Fourier transform (FFT). Left panel: chemisorption of 0.5 ML Co/Si(111)7x7. Data and FFT for normal incidence (continuous line) and grazing incidence (dotted curves). Right panel: CoSi₂ standard (dashed curves) and epitaxial 2D-CoSi₂/Si(111) at normal incidence (continuous line) and grazing incidence (dotted curve).

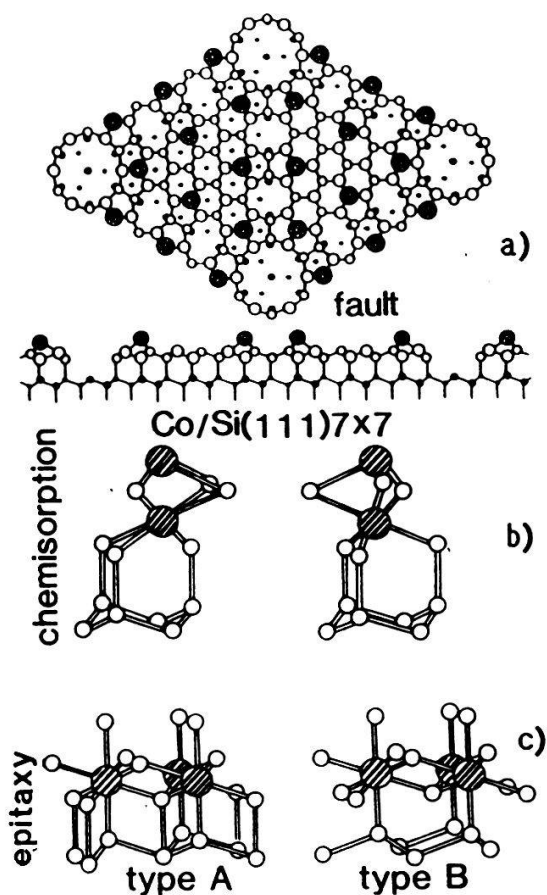


Fig.2 a) top and side view of the DAS model of Si(111)7x7. The cross hatched atoms are the Si adatoms. b) SEXAFS derived model for the chemisorption of Co (large hatched atoms) onto Si(111)7x7, both on unfaulted (left) and faulted (right) 7x7 sites. c) Hamann's models [5] of type A and B CoSi₂/Si(111) interfaces compatible with the SEXAFS results on the annealed samples.