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Determination of the atomic structure of the epitaxial $CoSi_2$:Si(111) interface using high-resolution Rutherford backscattering

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High-resolution Rutherford backscattering is employed to study the atomic structure at the epitaxial $CoSi_2$:Si(111) interface. The Si atoms of the substrate are found to bond to Co atoms in the silicide. In this bonding arrangement the interface Co atoms are fivefold, or possibly eightfold, coordinated. Bond-angle distortions are essentially absent.

I. INTRODUCTION

Epitaxial silicide-silicon heterostructures offer a unique possibility for studying the correlation between the structural and electrical properties of metal-semiconductor interfaces. Knowledge of the crystallography at the interface is decisive for understanding the energetic barrier for carrier transport across the interface (Schottky barrier). Lateral carrier transport in very thin $CoSi_2$ layers appears not to be affected by size effects because of the structural perfection of the $CoSi_2$:Si(111) interface.[1] The aim of this paper is to provide a detailed structure analysis of the $CoSi_2$:Si(111) interface.

The metal silicide $CoSi_2$ has a face-centered-cubic unit cell with the CaF_2 structure. The $CoSi_2$ unit-cell side is smaller than that of Si by 1.2% at 293 K, indicating a good match for epitaxy. The most commonly observed epitaxial relationship with Si(111) is one in which the silicide film is (111) oriented but 180° rotated about the substrate normal, labeled as type-*B* epitaxy.[2] The silicide may also have the same in-plane orientation as the Si(111) substrate (type *A*). In modeling the corresponding atomic structures of the interface there are two distinct possibilities: The Si dangling bonds of the substrate may either be attached to the Co atoms or to the Si atoms in the silicide. Figure 1 shows for a type-*B* film the corresponding bonding arrangements at the interface. The two models are distinguished by the coordination number of the last metal atom in the silicide adjacent to the Si substrate. In the case of a Co-Si bond across the interface the coordination number is 5, or possibly 8. A Si—Si interface bond results in sevenfold-coordinated Co atoms at the interface. The *B*-type $CoSi_2$:Si(111) interface has previously been examined by cross-section transmission electron microscopy (TEM) and x-ray standing waves (XSW). From high-resolution TEM lattice images Gibson *et al.*[3] concluded that the fivefold-interface model is the most likely one, but an unambiguous structure assignment could not be made. Recently we presented a measurement of the interplanar distance at the interface by the use of synchrotron-excited XSW's.[4] An interface distance consistent with the fivefold model was measured and the bonds across the interface were found to be slightly dilated.

Here we address the question whether atomic positions at the $CoSi_2$:Si(111) interface are indeed in accordance with the fivefold model, and search for possible bond-angle distortions at the interface. The atomic positions are determined using high-resolution Rutherford backscattering spectrometry (RBS) with the use of focusing effects.[5,6] With this technique it is possible to penetrate an overlayer and to probe the location of interface atoms with monolayer sensitivity. Our results show that the Co atoms indeed bond to the Si substrate, i.e., the Co atoms at the interface are fivefold (or eightfold) coordinated. The sevenfold model is ruled out. This finding is in striking contrast with the results obtained on the isomorphous, type-*B* $NiSi_2$:Si(111) system, for which various techniques agree on it having sevenfold-coordinated atoms at the interface.[6–8]

The experimental method is described in Sec. II. Details concerning sample preparation and the experimental setup are given in Sec. III. In Sec. IV the ion scattering measurements are presented and in Sec. V the interface structure is derived from the results. Our results are summarized in Sec. VI.

II. METHOD

Figure 1 shows schematically the scattering geometry which was used to distinguish between the two structure models of the type-*B* $CoSi_2$:Si(111) interface. At this stage, the distinction is made only between the fivefold and the sevenfold interface structure. High-resolution RBS has been explained elsewhere;[9] only the relevant aspects will be discussed here. A parallel ion beam is aligned with the $[00\bar{1}]$ channels in the silicide. Ions impinging close to an atomic row are deflected away from their original direction. As a consequence, the initially uniform flux distribution is focused into a strongly peaked one. The lateral position of the focus within the channel can be varied by slightly changing the incidence angle α of the ion beam. Upon entering the substrate, the focused ion flux may hit the substrate atoms marked 2–5 in Fig. 1. Deeper atoms in the substrate are shadowed by these atoms, while atom 1 is shadowed by the atomic rows in the silicide. The consequence of trajectory focusing is shown in Fig. 2. The figure displays, as a function of α, the hitting probabilities of atoms 2–5 as calculated with Monte Carlo simulations[10] (see also Sec. V). The hitting probabilities of the various interface atoms change by almost 2 orders of magnitude as the angle of incidence α is changed. Atoms 4 and 5 are hit and atoms 2 and 3 are shadowed if $34.8° < \alpha < 35.1°$. An increase of α by only 0.6° reverses this situation. This holds for both the fivefold and the sevenfold structure. The hitting probability for a surface atom is unity by definition.[9] Because of focusing, the hitting probability of an interface atom may be far in excess of unity (see Fig. 2).

In Fig. 1 the ingoing and outgoing paths of the ions are sketched for the case that atoms 4 and 5 are fully hit ($\alpha = 34.8°$). Ions backscattered from the interface atoms emerge from the $CoSi_2$ [110] channels within a well-defined range of exit angles β. For the fivefold structure the location of atoms 4 and 5 with respect to these channels is such that this angular range is very broad. For the sevenfold structure, the angular range of the backscattering yield is much narrower. When α is increased so that atoms 2 and 3 are probed, the situation is the opposite: then the angular range for the sevenfold structure is much wider than for the fivefold structure. Thus, in order to differentiate between the fivefold and sevenfold interface structures, the angle-dependent backscattering yield from the Si atoms at the interface is measured for different incidence angles of the beam about the $[00\bar{1}]$ axis of the silicide.

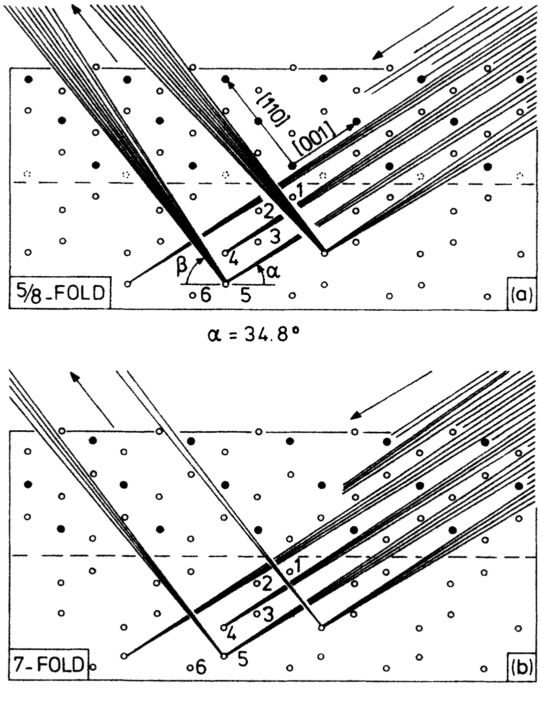

FIG. 1. Scattering geometry used for determination of the type-*B* $CoSi_2$:Si(111) interface structure, showing $(1\bar{1}0)$ planes with (a) fivefold- (or possibly eightfold-) and (b) sevenfold-coordinated Co atoms at the interface. Open and solid circles represent Si and Co atoms, respectively. For the eightfold coordination, the interface comprises the Si atoms denoted by dashed circles in (a). α is the angle of incidence and β is the exit angle.

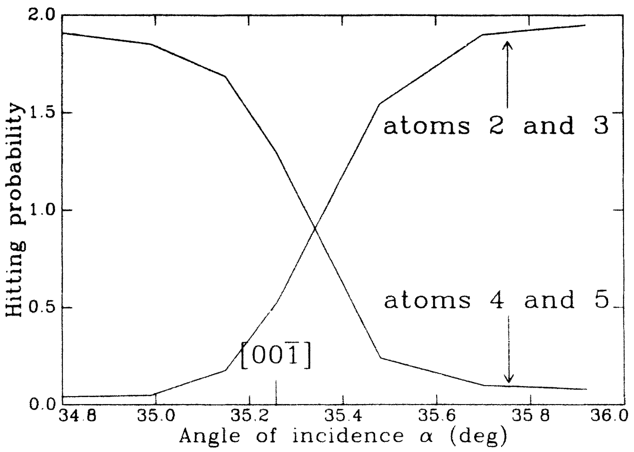

FIG. 2. Simulated hitting probabilities for interface atoms 4 and 5, and 2 and 3, as a function of angle of incidence α for 98-keV H^+ ions incident along the $[00\bar{1}]$ silicide direction. The silicide thickness is 27 Å.

The success of the above method critically depends on the action of the overlayer as an ion lens. Good crystallinity of the silicide overlayer is a prerequisite for the focusing to occur at all. Secondly, the ions need to be focused onto the equilibrium positions of the interface atoms. By carefully choosing the experimental conditions the latter requirement can be fulfilled. We note that the focusing effect employed here is distinctly different from the classical channeling effect.[11] In the channeling process, the trajectories of the ions entering the crystal oscillate with a wavelength λ and eventually get out of phase relative to one another. This situation of statistical equilibrium[11] results in a depth-independent spatial distribution in the channel, which is peaked in the center. Here the initially in-phase oscillatory motion along the channel axis causes the increase of the hitting probability of the interface atoms. Focusing of the ions occurs at a trajectory length of $\lambda/4$. For an axial-symmetric channel, the wavelength is given by

$$\lambda = 2\pi\sqrt{E/k} \;, \qquad (1)$$

where E is the ion energy of the incoming ion beam and k a constant for a given channeling direction.[12] Thus the thickness of the silicide overlayer and/or the primary energy of the ion beam can be varied to achieve optimal focusing conditions.

III. EXPERIMENT

The experiments were carried out in a multichamber ultrahigh-vacuum system, consisting of a surface analysis chamber, a molecular-beam epitaxy (MBE) apparatus and a sample loading chamber.[13] Samples were *in situ* grown and analyzed. The base pressure is 7×10^{-9} Pa. During deposition and sample transport the pressure rose to 7×10^{-8} Pa.

The high-resolution RBS experiments were performed in the analysis chamber which is coupled to a 200-kV ion accelerator. A beam of 98-keV protons collimated to within 0.1° was directed onto the sample. Since the silicide is extremely sensitive to ion-beam damage, protons are preferred over He ions.[14] The backscattered protons are energy analyzed with a toroidal electrostatic analyzer, which enables simultaneous detection over a 14° range of scattering angles. The direction of minima and maxima in the angular backscattering yield can be determined very accurately (to within 0.05°) with respect to the direction of the [110] axis in the silicide. Combining the energy resolution of the analyzer ($\Delta E/E = 4\times10^{-3}$) with the inelastic energy loss of ions traveling through the silicide film [54 eV per Å-depth interval for 98-keV H^+ in the scattering geometry of Fig. 1 (Ref. 15)], we obtain a depth resolution of 7 Å. By use of well-known calibration procedures backscattered intensities were converted into the effective number of monolayers visible to beam and detector.[9] The accuracy of the conversion is better than 5%. The sample orientation is controlled by a three-axis goniometer, thus allowing for alignment of the ion beam with respect to the silicide channels to within 0.05°.

The Si(111) substrate ($8\times16\times0.38$ mm^3 in dimension) was cleaned by mild sputtering and annealing.[16] After cleaning no impurities were detected by either Auger-electron spectroscopy [$I(\mathrm{C}(KLL))/I(\mathrm{Si}(LVV))$ and $I(\mathrm{O}(KLL))/I(\mathrm{Si}(LVV))$ intensity ratios $<1\times10^{-3}$ in the differentiated spectrum] or ion scattering (detection limit 10^2-10^{-3} monolayer for elements heavier than Si). The integrated area of the clean Si surface peak measured with the ion-beam channeling in the $[\bar{1}\bar{1}1]$ direction, and the detector centered about the [001] blocking direction, was equal to the value for a Si(111)-(7×7) surface.[17]

The $CoSi_2$ overlayer needs to be uniform without the presence of pinholes for a sound structure determination of the interface by RBS. A novel solid-phase epitaxy technique was employed to avoid pinhole formation.[18] Co was deposited at room temperature on the clean surface by sublimation from resistively heated pure Co wires. The amount deposited was 7.1×10^{15} Co atoms/cm^2. The unreacted Co film was covered with a thin layer of Si with equal thickness. The resulting Si/Co/Si(111) sandwich was subsequently annealed at 670 K for 180 s and reacted to a $CoSi_2$ layer of 27 Å thickness. With ion scattering and cross-section TEM it was verified that the silicide layers so obtained are essentially pinhole free (pinhole density $<10^5$ cm^{-2}) and have the correct stoichiometry.[18]

The $CoSi_2$ layers were found to be nonpseudomorphic and essentially free of strain.[4,18] The absence of tetragonal strain is deduced from accurate measurement of the directions of the main crystallographic axes in the silicide film. Apparently, the strain due to the misfit with the substrate lattice is relieved by the presence of misfit dislocations at the interface.

The $[00\bar{1}]$ channel of the silicide makes an angle of 35.26° with the surface. For a silicide thickness of 27 Å, the path length down to the interface atoms 2–5 is ~50 Å. From Eq. (1) it follows that protons of 98 keV have the desired quarter-wavelength of 50 Å. The presence of steps at the interface causes the location of the interface atoms along the ion trajectory to vary with ±16 Å. TEM micrographs show that the surface of the silicide is flat and that less than 30% of the interface area contains terraces of mainly three (111) planes in height. Occasionally steps of two planes associated with a misfit dislocation are observed.[18,19]

IV. RESULTS

A collection of energy spectra is shown in Fig. 3 for an angular range of the exit angle β of 14°. The angle of incidence α was set at 34.8°, so that atoms 4 and 5 are hit. Two distinct peaks are observed at 95 and 91 keV, corresponding to backscattering from Co and Si atoms in the silicide surface region. The hump indicates the yield of ions backscattered from Si atoms 4 and 5 at the interface and shows up in a limited range of exit angles near the [110] blocking minimum in the silicide. Due to the high-energy resolution of the detector, the interface signal is well resolved in energy from both the surface backscattering contribution and the steeply rising dechanneling background from the Si substrate at lower energies. The total interface yield at a given exit angle is obtained by integration over an energy window in the recorded spectra so that only ions backscattered from the interface are selected. To illustrate this procedure, we reproduce in Fig. 4 a single energy spectrum from Fig. 3, which was taken at the central exit angle ($54.8° < \beta < 55.6°$). The integration was performed over the hatched area. After correction for the Rutherford cross-section and neutralization efficiency, the integrated interface yield is converted to monolayer units. One monolayer is defined as 8.02×10^{14} atoms/cm^2.

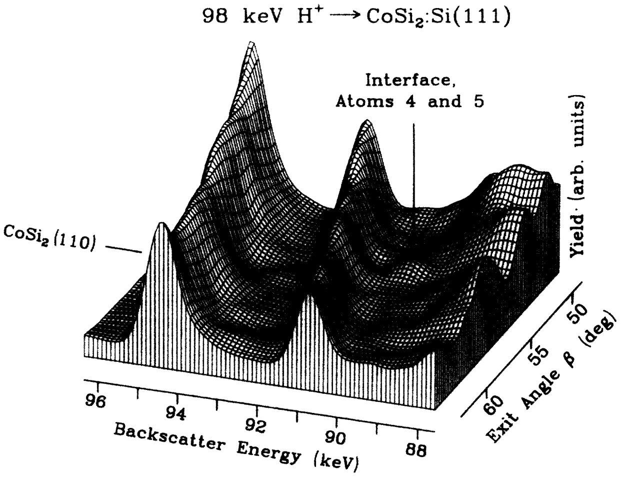

FIG. 3. Backscattering energy spectra measured in the scattering geometry of Fig. 1 in a 14° angular range around the [110] silicide axis. The angle of incidence α is 34.8°. Backscattering from Co and Si surface atoms results in two distinct surface peaks. The arrow points to the hump in the spectrum due to backscattering from interface atoms 4 and 5.

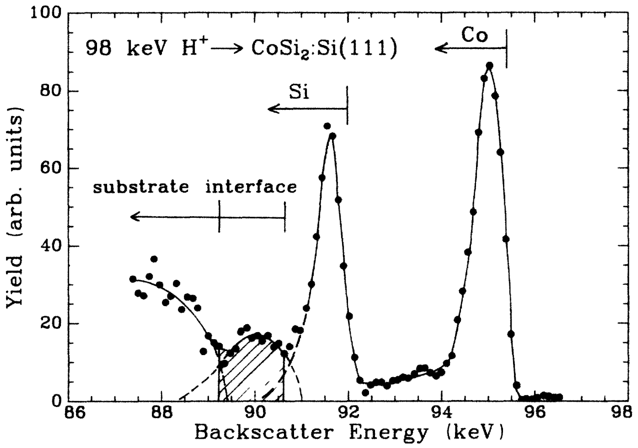

FIG. 4. Central energy spectrum of Fig. 3, for ions exiting within a 0.8°-wide cone around the [110] direction. The angle of incidence α is 34.8°. The solid curve serves to guide the eye. The integrated interface peak area is shown shaded.

Angular distributions of the interface yield around the [110] exit channel have been determined for three different angles of incidence: $\alpha = 34.8°$, 35.2°, and 35.5°. The results are shown in Fig. 5(a) as a function of exit angle β (solid points). In order to obtain a good match with the height of simulated angular distributions (solid curves), the three experimental distributions had to be multiplied by a factor of ~ 2 (see below). At $\alpha = 34.8°$, corresponding to atoms 4 and 5 being hit, the angular distribution is quite broad. With increasing angle α, the distribution sharpens up. This is precisely the behavior expected for a fivefold interface structure.

V. DISCUSSION

The atomic bonding arrangement at the interface has been analyzed in more detail by comparing the results with Monte Carlo simulations[10] for different structure models. In such a simulation $\sim 2\times 10^5$ ions are tracked through a slab of the bicrystal. The Molière approximation of the Thomas-Fermi scattering potential is used to calculate the small-angle deflections from the atoms.[20] The effective number of visible interface layers is acquired with the nuclear-encounter probability concept[21] and the principle of time reversal.[22] Lattice vibrations are modeled with an isotropic Gaussian-distributed probability density for the displacement of each atom from its equilibrium position. We are not aware of any experimental determination of the vibration amplitudes in bulk $CoSi_2$. Crude estimates based on electrical transport studies indicate that the difference in the Debye temperature of $NiSi_2$ and $CoSi_2$ is less than 100 K.[23] The one-dimensional rms vibration amplitudes of Co and Si are taken to be equal to the values used in an earlier study for Ni and Si in $NiSi_2$.[24] Our simulations demonstrate that the absolute interface yield and the angular distributions are not significantly affected by a change of 25% in the bulk vibration amplitudes.

The angular distributions simulated for the fivefold and sevenfold structures are compared in Figs. 5(a) and 5(b) with the experimental data. In the simulation the overlayer lattice was assumed to be free of defects and to be perfectly matched to that of the substrate. In addition, the bonds across the interface were assumed to be bulk-like for the sevenfold structure and for the fivefold structure a dilation of 0.05 Å was taken.[4] For the fivefold structure the simulations closely match the data as regards both angular shapes and positions, whereas for the sevenfold structure they do not at all. The latter structure is clearly ruled out.

With the aid of Fig. 1 and the Monte Carlo simulations, the shapes of the angular distributions are readily interpretable in backscattering contributions from the different interface atoms. Consider, for example, the angular distribution calculated for the fivefold structure and for incidence angles in the range $34.8° < \alpha < 35.0°$. This distribution is the sum of two shifted "emission cones" from atoms 4 and 5, and is therefore broad and structured [Fig. 5(a)]. The measured distribution is of about the same form but with rounded structures. For the sevenfold structure and the same α, the emission cone from atom 4 is calculated to be much narrower and to merge with the one from atom 5 [Fig. 5(b)]. This results in a sharply peaked structure, which in form deviates strongly from the observed angular distribution. For larger α, when atoms 2 and 3 are hit, the situation is essentially the reverse.

The absolute interface yields acquired from the Monte Carlo simulations were a factor ~ 2 higher than measured. (The measured yields plotted in Fig. 5 were multi-

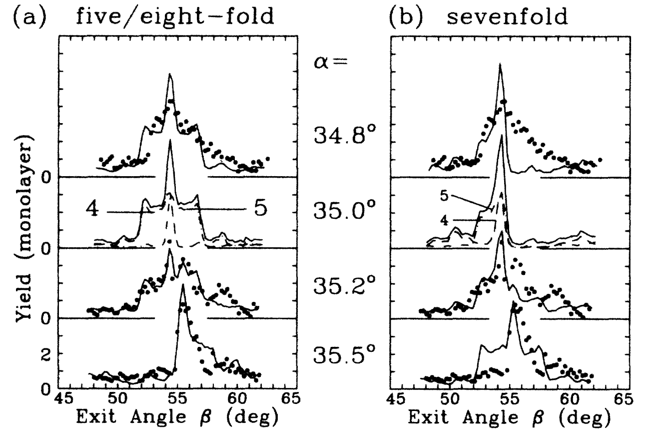

FIG. 5. Interface peak area as function of exit angle β recorded in the geometry of Fig. 1. Solid lines are results from Monte Carlo simulations and dots are experimental data. Panel (a) shows the simulations for the fivefold-interface structure, panel (b) for the sevenfold-interface structure. The dashed and dash-dotted curves indicate the backscattering contribution from atoms 4 and 5, respectively.

plied by this factor, so as to allow for a proper comparison with the simulated angular distributions.) Apparently, interface atoms 2–5 are much less visible to beam and detector than is expected on the basis of simulations for an ideal, defect-free, overlayer system. A reduction in visibility may be caused by defects in the overlayer, which scatter ions away from the focus. This, however, is not likely to influence the shape of the measured distributions. The presence of defects in the CoSi$_2$ layer is also evident from the rather high minimum yield measured behind the Co surface peaks in the energy spectra (see, e.g., Fig. 4) and from XSW analyses of similarly prepared overlayers.[4] A lower interface yield than expected may also relate to our method of peak integration in the energy spectra. The steps at the interface produce a lateral variation in the overlayer thickness. Consequently, the interface peak is broadened and has tails extending below the Si surface peak and the substrate background (Fig. 4). The tail regions had to be left out of the integration because their form is not known. The lateral variation in layer thickness also causes a smearing of the focusing distance, resulting in a reduced interface peak intensity.

The present data show that Co atoms of the silicide are attached to Si atoms in the substrate, but there are still two possibilities left for the coordination of the Co atoms at the interface. Besides the fivefold-coordination model, a model with eightfold-coordinated Co atoms at the interface can be constructed if the requirement of fourfold coordination for Si atoms is dropped at the interface. The eightfold model comprises an extra plane of Si atoms at the interface on silicide-lattice positions [Fig. 1(a)]. These Si atoms form three bonds with first-layer Co atoms and have one unsaturated bond. Since the equilibrium positions of the atoms are aligned with the $[00\bar{1}]$ silicide rows it is not possible to detect these atoms in the scattering geometry used. It is noteworthy that the earlier mentioned XSW is also insensitive to the presence of these atoms.

Finally, we consider possible bond-angle or bond-length relaxation at the interface, which would result in a rigid laterally and/or vertically translated overlayer lattice. A small outward displacement of the overlayer by 0.05±0.03 Å has been determined with XSW.[4] Let us consider a possible lateral displacement. Since the $(1\bar{1}0)$ plane is a mirror plane, only an in-plane displacement of the silicide along the $[11\bar{2}]$ direction with respect to the substrate is possible. For such a displacement, the $(11\bar{2})$ silicide planes do not coincide with the $(11\bar{2})$ substrate planes. The translation alters the spatial density distribution of the focused ions at the interface. For example, in the geometry of Fig. 1(a) a translation along the $[11\bar{2}]$ substrate direction causes the hitting probability of atoms 2 and 3 to increase. Furthermore, the emission cone of the interface atoms into the [110] direction will be shifted in angle. Extreme sensitivity to this angular shift of the interface yield is obtained for an incidence angle of $\alpha = 35.5°$. The corresponding distribution of the interface yield is reproduced in Fig. 6, together with Monte Carlo simulations for lateral displacements ΔY of the silicide film by −0.1 Å, 0 Å and +0.1 Å. Here a translation is defined to be positive in the $[11\bar{2}]$ direction. The best fit is obtained for no translation to within 0.05 Å. Similar analyses of other angles of incidence give identical results. These observations imply that the bond angles at the interface are essentially bulklike. On the basis of cross-section TEM micrographs of a Si:CoSi$_2$:Si heterostructure, d'Anterroches *et al.*[25] concluded that there was a translation $\mathbf{t}=\frac{1}{10}[01\bar{1}]$. Not only is the perpendicular bond dilation of 0.62 Å associated with such a translation incompatible with the XSW result,[4] but the lateral component is also at variance with the present data. The fact that the structure assignment by d'Anterroches *et al.* is not based on lattice image calculations makes their conclusions doubtful.

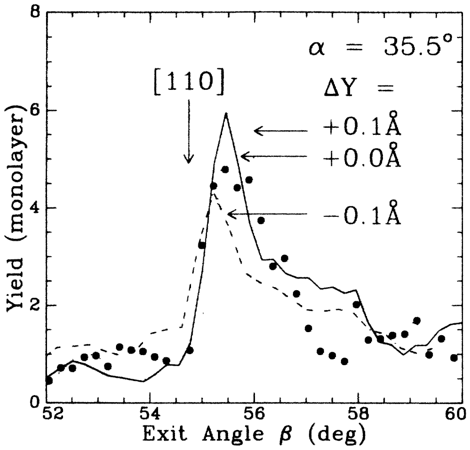

FIG. 6. Interface peak area as a function of exit angle β. The angle of incidence α is 35.5°. The data points (solid circles) are reproduced from Fig. 5. The curves are results of Monte Carlo simulations for parallel displacements of the silicide of −0.1, 0.0, and + 0.1 Å.

VI. CONCLUSION

The atoms at the epitaxial CoSi$_2$:Si(111) interface are arranged such that Si atoms in the top layer of the Si(111) substrate are bonded to the Co atoms in the silicide. Bond-angle distortions at the interface are essentially absent and the silicide overlayer is unshifted along the $[11\bar{2}]$ parallel direction with respect to the substrate. From the data presented here we derive a structure model which has fivefold- (or possibly eightfold-) coordinated Co atoms at the interface. This interface structure is in excellent agreement with earlier indications based on XSW (Ref. 4) and TEM (Ref. 3). For the NiSi$_2$:Si(111) system it was found that the interface bond is a Si—Si bond, i.e., the metal atoms are sevenfold coordinated.[6,7,8] This contrast between CoSi$_2$ and NiSi$_2$ is puzzling. Very recently, quantum chemical cluster calculations have been performed, which provide an explanation for the different bonding geometry of the two interfaces.[26]

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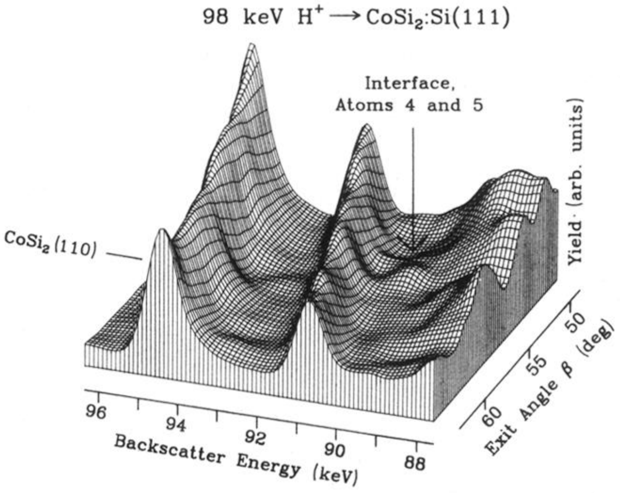

FIG. 3. Backscattering energy spectra measured in the scattering geometry of Fig. 1 in a 14° angular range around the [110] silicide axis. The angle of incidence α is 34.8°. Backscattering from Co and Si surface atoms results in two distinct surface peaks. The arrow points to the hump in the spectrum due to backscattering from interface atoms 4 and 5.