New interface structure for *A*-type $CoSi_2$/Si(111)

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A new model of a $CoSi_2$/Si(111) interface structure has been generated using images produced by *Z*-contrast scanning transmission electron microscopy. The images indicate that the top and bottom interfaces between the type-*A* buried $CoSi_2$ layer and Si(111) both have eightfold coordinated Co atoms. This is accomplished by converting the one interface structure from sevenfold to eightfold coordination by locating a twinned layer of Si at the interface. The preference for this interface over the sevenfold type-*A* structure is in agreement with theoretical predictions.

Because of their small lattice mismatch and similar structures, single-crystal cobalt and nickel disilicide films can be grown with relative ease in contact with Si. These well-defined couples have attracted much interest because of their technological importance and because they appear to be model systems for studies of a range of interface properties, including the correlation between atomic structure and Schottky barrier height (SBH). Many possible structures for the disilicide/Si(111) interface have been proposed.[1,2] They have been classified according to two criteria: the coordination of the metal atoms at the interface and the relative orientation of the disilicide and Si crystals. If one assumes the two crystals join along flat bulk terminated {111} surfaces, the silicon substrate binds either to the metal atoms at the interface, leading to eightfold coordinated metal atoms everywhere, or to the silicon atoms of the silicide, leading to sevenfold coordinated metal atoms at the interface [see Fig. 1(a)]. The disilicide films can have the same crystallographic orientation as the Si substrate (type-*A*) or a twin orientation in which the film is rotated 180° about the [111] surface normal (type-*B*).

It has been shown that $CoSi_2$ and $NiSi_2$ films can be grown with either orientation by controlling the growth conditions.[3–5] Both theory[6,7] and experiment[1,8] have determined that the coordination of the Ni atoms at both *A*- and *B*-type interfaces is sevenfold. Type-*B* $CoSi_2$/Si(111) interfaces show evidence for eightfold coordinated Co,[9,10] in agreement with theoretical predictions.[6,7] However, high-resolution phase contrast images of the type-*A* interface have been interpreted as evidence of sevenfold coordinated Co.[10]

Clearly, the understanding of the Schottky barrier height (SBH) would greatly benefit from additional experiments on these systems with homogeneous interfaces using techniques to access the buried interface and provide detailed and directly interpretable structure characterization. In this study, the atomic structure of $CoSi_2$/Si interfaces of buried layers formed by a Co implantation was characterized by high-resolution *Z*-contrast imaging. In this imaging mode, each atomic column can be imaged independently with high compositional sensitivity.[11] These images clearly reveal a new structure for the $CoSi_2$/Si(111) interface that does not appear to have been considered in previous x-ray or electron microscopy investigations. The intensity displayed in these images is collected with an annular dark field detector in a VG HB501 UX scanning transmission electron microscope. With the detector angles used, it has been found that each atom (or small packet of atoms) can be considered to scatter independently with a cross section that approaches the atomic number squared dependence of Rutherford scattering.[11] The image depends on the local intensity illuminating each atom; thus when the atomic columns parallel to the electron probe are separated by more than the 0.22 nm probe size, the columns can also be illuminated individually, giving a direct image of the positions of the projected atomic columns with high compositional sensitivity. Because there are no contrast reversals, these columns are unambiguously identified as bright features in the image. The incoherent nature of the *Z*-contrast image makes it ideal for analysis of unknown structures. Model structures are obtained by direct inspection of the image rather than from preconceived trial structures, making the technique sensitive to unanticipated structures.

The buried $CoSi_2$ layer was produced by implanting Co^+ ions (200 keV, 2×10^{17} ions/cm^2) in Si(111) substrates heated to 350 °C. Following implantation, the substrates were

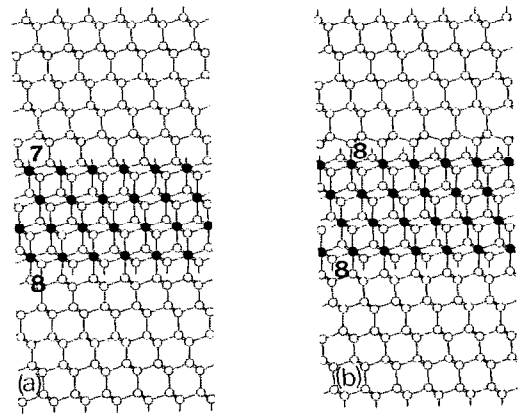

FIG. 1. Models of the atomic structure of an aligned type-*A* buried $CoSi_2$ layer in Si as projected along the [01$\bar{1}$] direction (a) Structure without any modifications. The top (111) interface has sevenfold coordinated Co atoms and the bottom interface has eightfold coordinated Co atoms. (b) Structure with the observed twinned interfacial Si layer at the top interface (111). Both interfaces have eightfold coordinated Co atoms.

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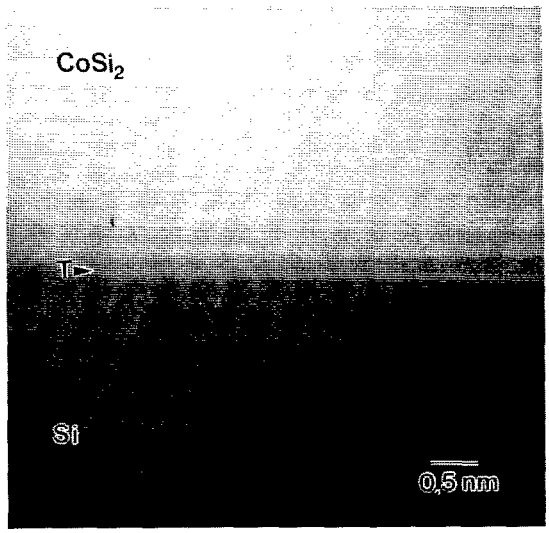

FIG. 2. Z-contrast image of a section of the $CoSi_2$/Si(111) interface projected along the [0-11] direction showing a twinned interfacial layer of Si. Although the {111} shifts across the interface are consistent with the sevenfold coordinated interface in Fig. 1(a), the actual interfacial Co coordination is eightfold. The orientation of the disilicide relative to this twinned layer is type-B.

capped with 200 nm of SiO_2 and then given a two-step anneal in high purity argon (750 °C for 30 s+1150 °C for 10 s). This treatment results in a continuous, buried $CoSi_2$ layer ~70-nm thick, ~90 nm below the substrate surface. Cross-section specimens were prepared in the {110} orientation by mechanical polishing to 10 μm and ion milling with 2–5 keV Ar^+. The atomic structure of the $CoSi_2$/Si interfaces were characterized by high-resolution Z-contrast imaging using a VG Microscopes HB501 UX scanning transmission electron microscope operating at 100 kV.

The Z-contrast images of the [110] projection of the $CoSi_2$/Si(111) interface presented in Fig. 2 strongly suggest a possible interface structure not previously considered. Neglecting for the moment the interface, the $CoSi_2$ and Si lattices have the same orientation (type-A) as indicated by the parallel {111} and {110} planes on the two sides of the interface. The shifts of the {111} planes across the interface are consistent with the interface model where the Co at the boundary has sevenfold coordination. But this direct image shows that there is a fault in the stacking of the Si crystal at the interface. The interfacial Si layer is rotated 180° around the [111] surface normal. Therefore, those Si atoms in contact with the disilicide have the twinned type-B orientation. From the position of this twinned layer of Si relative to the interfacial Co layer, it is determined that the Co coordination is eightfold at this interface as it is in the bulk.

This feature is not always obvious in a phase contrast image because it can be masked by interference generated between the two crystals as demonstrated in Fig. 3. The discontinuity at the interface leads to intensity variations, which can only be modeled by image simulations of predicted structures. Therefore, the method of interpretation of the phase contrast images has relied on the (111) fringe shifts across the interface. As seen in the simulated phase contrast image in Fig. 3, the presence of a twinned layer of Si at the interface could easily be missed. With the Z-contrast technique there is a direct connection between the image and the actual structure; and thus, the correct structure can be deduced intuitively from the image. Phase contrast simulations based on the new structure deduced from Z-contrast microscopy produce images consistent with experimental phase contrast results.[10,12,13]

The continuous buried disilicide layer forms through coalescence of distinct precipitates.[14] Consider the formation of a parallel-sided precipitate as shown in Fig. 1. Assuming no defects are introduced, if one interface has eightfold coordinated metal atoms, the opposite interface must have sevenfold coordinated metal atoms. This is also true for type-B layers. There should be no difference between a buried precipitate and a buried continuous layer formed by implantation. The geometric constraints on the two morphologies are identical. Conversion to a structure where both interfaces are sevenfold (or eightfold) could be accomplished with the addition (removal) of a row of Si atoms.[15] It has been reported that both interfaces for B-type buried layers appear to be eightfold coordinated, while type-A buried layers appear to have two sevenfold coordinated interfaces.[10] The interfacial twin we observe allows eightfold Co coordination at both interfaces between the type-A oriented buried $CoSi_2$ layer and the Si matrix. It is expected that the new interfacial structure is present along a fraction of both the top and bottom interfaces, with the normal type-A eightfold coordinated structure at the opposite interface. Unfortunately, it was not possible to obtain high-resolution images from the top and bottom interfaces of the same region of the buried layer in order to confirm the model in Fig. 1(b), although, regions of normal untwinned type-A interface were observed (Fig. 4), and only these two interface structures were observed in the samples examined. They appear in alternating patches along both the top and bottom interfaces.

These results indicate that the type-A buried $CoSi_2$ layer in Si(111) has the same combination of two different atomic structures at the top and bottom interfaces. Both interface

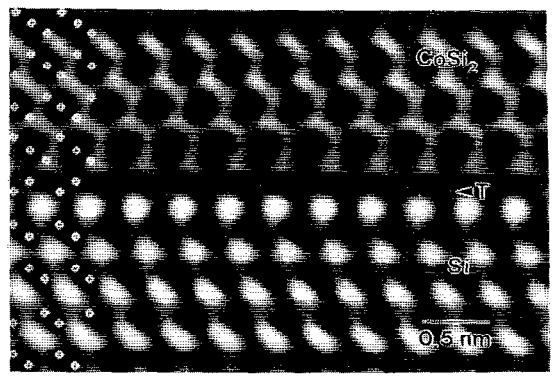

FIG. 3. Simulated phase contrast image of the new interface model with the twinned layer of Si (200 kV, C_s=1.3 mm, defocus=−50 nm, thickness=10 nm).

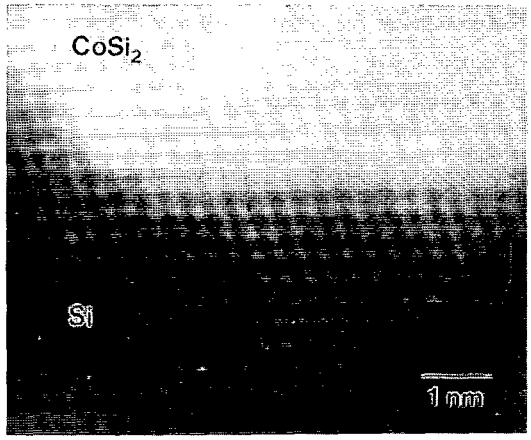

FIG. 4. Z-contrast image of the (111) interface between a type-A $CoSi_2$ layer and Si without the twinned interfacial layer. The Co coordination at this interface is eightfold. This is the structure of the bottom interface in the model of Fig. 1(a).

structures have eightfold coordinated Co atoms. This is accomplished by converting the one interface structure from sevenfold to eightfold coordination by locating a twinned layer of Si at the interface. From Z-contrast imaging, we find that what was thought to be a type-A (111) interface with sevenfold coordinated metal atoms, actually, on the atomic scale, is a type-B interface with eightfold coordinated metal atoms. The preference for this interface over the sevenfold type-A structure is in agreement with theoretical predictions.[6,7] Very similar Schottky barrier heights for top and bottom diodes have been measured on similarly prepared samples.[16]

We have generated a new model of the $CoSi_2$/Si(111) interface using images produced by the Z-contrast technique. These results are a very clear demonstration of the ability to directly image and interpret unforeseen structures with the Z-contrast technique. It is expected that further work will lead to new levels of insight into the important and controversial relationship between the atomic structure and electronic properties.

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