Misfit dislocations at the CoSi\textsubscript{2}/Si (001) interface studied by aberration-corrected high angle annular darkfield imaging.

Meiken Falke, Uwe Falke, Andrew Bleloch
UK SuperSTEM, Daresbury Laboratory, Daresbury WA4 4AD, United Kingdom
E-mail: m.falke@physik.tu-chemnitz.de

Abstract. Epitaxial cobalt disilicide thin films buried in (001) silicon were grown by annealing a precipitate distribution in a nearly undisturbed Si matrix. The CoSi\textsubscript{2}/Si junction was studied by dedicated aberration-corrected scanning transmission electron microscopy. Earlier, we unequivocally identified two different interface structures, the atomic arrangement and frequency of appearance of which are consistent with predictions from total energy calculations. This paper is dealing with the interface dislocations in more detail. Due to the cubic crystal symmetry of both, the silicide and the Si substrate, the interface consists of a patchwork of different domains, which are rotated to each other by 90°. Dislocations are required at the boundaries of those domains. Additionally, misfit dislocations are expected, since under the applied conditions for non-pseudomorphic growth a relaxed interface is formed. A complex defect structure at the interface domain boundaries, always associated with \{111\}-facets was found to solve both constraints, thereby minimising the interface energy of the system efficiently.

1. Introduction
The CoSi\textsubscript{2}/Si-junction has been a model system for understanding Schottky contacts for decades. The CaF\textsubscript{2} type lattice (Fm\textsubscript{3}m) of CoSi\textsubscript{2}, which is similar to the diamond structure of Si (Fd\textsubscript{3}m) with a lattice mismatch of $\Delta a = (a_{\text{silicide}} - a_{\text{silicon}})/a_{\text{silicon}} = 1.2\%$ allows atomically smooth conductor/semiconductor junctions to be generated by epitaxial growth on silicon. A strong influence of the local interface structure on the Schottky barrier height was shown theoretically [1] and suggested by experimental results [2, 3]. A considerable amount of work has been done [4, 5, 6, 7, 8] to understand the local interface structures. But, a complete and unambiguous determination of the local atomic arrangement at the CoSi\textsubscript{2}/Si interface was only possible utilizing aberration corrected high angle annular darkfield imaging in a dedicated STEM [9, 10]. Two different interface structures have been determined. A (2×1) reconstructed one comprising seven-fold coordinated Co atoms was observed frequently. An unreconstructed one, comprising eight-fold coordinated Co [10] was observed less often. For symmetry reasons each interface structure can appear in two domains, which differ in height along [001] by one atomic layer and in rotation by 90°. The CoSi\textsubscript{2}/Si interface is a patchwork consisting of those domains. The complex defects at the domain junctions, will be described.
2. Experimental
Epitaxial CoSi$_2$ films buried in silicon by Allotaxy [11] were used to study the structure of the CoSi$_2$/Si interface. The chosen film formation conditions result in non-pseudomorphic growth. That means lattice distortions are expected in order to accommodate the buried continuous epitaxial CoSi$_2$ film with its 1.2% smaller lattice constant in the Si-matrix. The lower silicide silicon junction, facing the substrate wafer side, was chosen for investigation, since it provided extended smooth interface areas [10] (figure 1).

Electron transparent cross-section samples for the [110] zone axis were prepared by tripod polishing followed by 10-15 minutes low angle ion milling at 3 kV in a Baltec RES10.

The HAADF signal increases monotonically with the atomic number of the scattering atoms, provided the sample thickness is suitable and not changing rapidly within the scanned area and the silicide/silicon interface in question is smooth [12, 13]. Aberration correction routinely allows a probe size of about 0.1 nm to be used. This in combination with HAADF imaging in [110] zone axis of the junction provides the tool to unequivocally distinguish atomic columns consisting of purely metal or silicon respectively. The atomic arrangement directly at the interface can be derived straightforwardly from the HAADF images, given, that all atomic columns investigated there in [110] zone axis, are also occupied purely by either the metal or the silicon.

The electron microscopy was carried out using a dedicated STEM VG-HB501 equipped with a Nion-MarkII-C$_s$-corrector [14, 15]. The microscope was operated at 100 keV with a 0.1 nm scanning probe, a 24 mrad probe convergence angle and an angular acceptance range of the HAADF detector of (70-210) mrad. The presented images were not processed. To visualise the atomic models the program Mercury [16] was used.

3. Results and Discussion
To understand distortions at the silicide silicon junction, it is first necessary to describe the atomic arrangement of the undisturbed interface parts.

Figure 2 shows ball and stick models of the two found and determined interface structures. In [110] zone axis of the silicon substrate two $<110>$ type projections of each interface, rotated by 90° can be found. As can be easily seen from the models in figure 2 and crystallographic considerations [17], dislocations are required at the junction of each combination out of two of them. The corresponding minimum Burgers vectors are of the $1/4<111>$ type for most of the configurations [10]. Since the {111} planes are the growth planes in the CoSi$_2$/Si system, the interface domain junctions can be expected to be {111}-planes as well. That means, with high
certainty, imaging in the [110] zone axis of a thin sample will provide the view along smooth interface domain boundaries so that the contrast will not be obscured by further structure changes in the viewing direction.

Now we can move on to an additional issue at relaxed interfaces of two similar structures, namely misfit dislocations. Since the CoSi$_2$ lattice constant is smaller than that of silicon, additional (110) planes will have to be added on the the silicide side of the interface at regular distances (15 nm in this case, assuming the relaxation of all in plane stress). In our experiment, additional CoSi$_2$ (110) planes accommodated at the interface to the silicon matrix were found about every 10-30 nm, indicating a relaxed film. The misfit dislocations were always associated with \{111\}-facets of different extension ranging from one up to several atomic layers in [001] direction (figure 3). Furthermore, at facets larger than one atomic layer in [001] direction, B-type micro-twins of one or two monolayers thickness and single columns of Si were found. The HAADF contrast related to smooth periodic interface structure was observed to be always different on each side of such facets, which means on each side of the extra (110) silicide plane.

![Figure 3. Two examples of the complex defect structure revealing a 1/4<111> type Burgers vector, additional planes are marked ([110] zone axis in Si).](image)

Apparently, the interface misfit dislocations are pinned to the junctions of interface domains, which in turn seem to be of rectangular shape in the (001) interface plane and matching in size the necessary equilibrium distance of the misfit dislocations.

Generally, at the epitaxial interface of a crystalline film with a slightly smaller lattice constant than the substrate, a continuous shift of lattice planes against each other needs to be accommodated with the lowest possible energy cost. In the relaxed case this is realised by a network of defects. We propose that the complex defects found at \{111\} facets, in particular the incorporated B-type micro-twins, single atomic silicon columns and large lattice openings, enable a certain flexibility for lattice compression or expansion in directions parallel to and in the (001) interface plane, so that the size of undisturbed interface domains can be maintained fitting to the equilibrium distance of misfit dislocation. Actually, it is not surprising, that merging them together into this complex defect structure, can solve several crystallographic constraints. Even interface steps due to wafer miss-cut or insufficient annealing time can be incorporated. The atomic arrangement at the edges of the \{111\} facet can not be interpreted straightforwardly from the HAADF contrast. Theoretical approach is required here to understand which stable atomic arrangement is possible after relaxation.
4. Summary
Our experimental data reveal the real interface structure in non-pseudomorphically grown cubic silicide/silicon systems.

A complex defect arrangement at the CoSi$_2$/Si interface was described on an atomic level. It was found to resolve lattice constraints due to misfit, growth conditions and domain formation at once, thereby minimising the systems energy efficiently. The result gives a deeper understanding of epitaxial growth with profound basic implications for practical thin film growth experiments.

For the CoSi$_2$/Si system it has to be pointed out, that under non-pseudomorphic growth conditions, even assuming sufficient annealing time and perfectly cut substrate wafers, the CoSi$_2$/Si-junction is very likely to always consist of a patchwork of different rotated interface domains, which at their boundaries incorporate additional silicide planes and require at least $1/4<111>$ type dislocations. Electrical properties of relaxed films will therefore resemble a net effect of locally very different interface structures separated by a network of defects. In case of fully pseudomorphic growth by other means than Allotaxy, the epitaxy of single large interface domains in a then much thinner and strained film might be possible.

5. Acknowledgements
The authors are grateful to the Engineering & Physical Sciences Research Council for funding the UK superSTEM facility at Daresbury Laboratory and would like to thank G. Baumann and K. Werner for careful TEM sample preparation and the Surface and Inteface Physics group at the University of Technology Chemnitz (Germany) for providing the Allotaxy samples.

6. References
[1] B D Yu, Y Miyamamoto, O Sugino, A Sakai, T Sasaki, T Ohno 2001 J. Vac. Sci. Technol. B 19 1180
[2] H v Känel, T Meyer, H Sirringhaus, E Y Lee 1997 Mut. Sci. Rep. RITU A 44 157
[3] Shiyang Zhu, R L Van Meirhaeghe, C Detavernier, F Cardon, Guo-Ping Ru, Xin-Ping Qu and Bing-Zong Li 1999 Solid-State Electronics 44 663
[4] D Loretto, J M Gibson, and S M Yalisove 1989 Phys. Rev. Lett. 63 298
[5] D Cherns, C J D Hetherington, and C J Humphreys 1984 Philos. Mag. A 49 165
[6] P Werner, W Jaeger, A Schueppen 1993 J. Appl. Phys. 74, 3846
[7] V Buschmann, L Fedina, M Rodewald and G Van Tendeloo 1998 Phil. Mag. Lett. 77 147
[8] M F Chisholm et al. 1994 Appl. Phys. Lett. 64 3608
[9] U Falke, A Bleloch, M Falke, St Teichert 2004 Phys.Rev.Lett. 92 116103
[10] M Falke, U Falke, A Bleloch et al. 2005 Appl. Phys. Lett. 86 203103
[11] S Mantl and H L Bay 1992 Appl. Phys. Lett. 61, 267
[12] S J Pennycook and D E Jesson 1990 Phys. Rev. Lett. 64 938
[13] E J Kirkland, Advanced Computing in Electron Microscopy ISBN 0-306-45936-1
[14] O L Krivanek, N Dellby, A R Lupini 1990 Ultramicroscopy 78 1
[15] [http://www.superstem.org](http://www.superstem.org).
[16] computer program Mercury, copyright by Cambridge Crystallographic Data Centre
[17] R C Pond 1998 Dislocations in Solids V8, ed F R N Nabarro, North Holland ISBN: 0444705155 pp 22