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# Properties of interfaces between cubic and hexagonal polytypes of silicon carbide

C Raffy, J Furthmüller and F Bechstedt

Institut für Festkörperteorie und Theoretische Optik, Friedrich-Schiller-Universität, 07743, Jena, Germany

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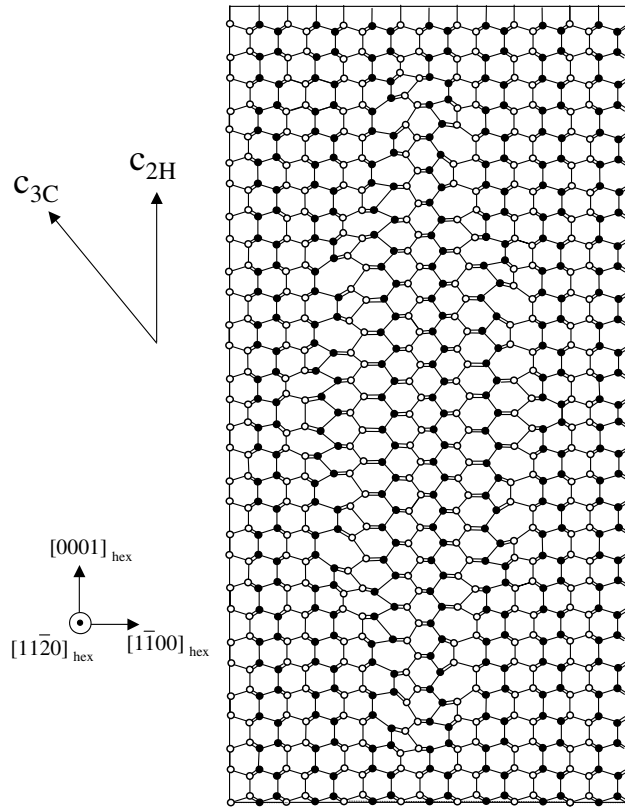
## Abstract

We present *ab initio* calculations of the properties of two types of interface between the cubic and hexagonal (wurtzite) polytypes of silicon carbide. The results are derived from density-functional calculations within the local-density approximation and the pseudopotential-plane-wave approach. We first study the interface along the (111) plane (corresponding to (0001) in the hexagonal representation) perpendicular to the stacking axis of the bilayers. Then we consider the interface along the (115) plane, which was already identified experimentally as a grain boundary in silicon and germanium. The (115) interfaces are especially interesting, since they may contribute to a quantum wire consisting of an inclusion of cubic SiC in hexagonal SiC. They are made up of five- and seven-membered atom rings and are free of dangling bonds. The cubic and hexagonal grains are tilted with respect to one another by an angle of  $38.94^\circ$ . In both cases of interfaces, the electronic properties are discussed. Whereas the (111) interface induces practically no states in the bulk fundamental gaps, the particular structure of the (115) interface generates a lot of states, resulting in a metallic behaviour.

## 1. Introduction

Stacking faults and grain boundaries are among the most important two-dimensional defects. In a crystal with stacking faults, the various lattice planes are not stacked in the same way as in the ideal crystal, but certain lattice planes are twisted by an angle. Grain boundaries occur in crystals which consist of two differently oriented half-crystals. The grain boundary is the lattice plane at which these two half-crystals meet.

Silicon carbide crystals are known to contain stacking faults. The combination of cubic and hexagonal stackings results in many polytypes [1, 2]. Stacking faults have been attracting a great deal of interest. Lendenmann's group [3] put the degradation of the electrical characteristics of bipolar SiC devices down to these faults. Lambrecht's group [4] also studied the impact of the stacking faults on electronic devices, and concluded that they show



**Figure 1.** A schematic model of a quantum wire consisting of an inclusion of a 3C crystal in a 2H matrix. The atoms with the same colour belong to the same  $(11\bar{2}0)$  plane. The structure of the interface is discussed in the text.

deterioration under long-time operation. However, polytypism also gives some advantages for constructing electronic devices, for example homomaterial heterostructures. Quantum wells can be made by embedding a SiC polytype in another polytype with a wider gap [5]. In figure 1, we show a schematic model of a quantum wire oriented along the  $[11\bar{2}0]$  direction consisting in a cubic (3C) crystal embedded in a hexagonal (2H) matrix.

In this paper, we investigate the properties of two interfaces between 3C- and 2H-SiC. We have proceeded by increasing the complexity of the interface. We first study the well-known (111) interface, which is perpendicular to the stacking axis of the bilayers and can be thought of as a stacking fault. This interface represents the usual cubic/hexagonal transformation in an fcc crystal, which is achieved by the shear of  $\frac{1}{6}[112]$  partial dislocations on every other (111) plane [6]. This mechanism changes the stacking sequence from ABCABC to ABABAB. The resulting orientation is  $(111)_{\text{cub}} \parallel (0001)_{\text{hex}}$ , and  $[1\bar{1}0]_{\text{cub}} \parallel [11\bar{2}0]_{\text{hex}}$ . Then, we study the interface between 3C- and 2H-SiC along the (115) plane, which occurs in the model of quantum wire of figure 1. This interface is a grain boundary which separates two crystals of different polytypes tilted by the angle of  $38.94^\circ$ . Instead of the usual six-membered rings, the interface region contains alternating five- and seven-membered rings, which allows one to keep the fourfold coordination. The cubic (115) plane coincides with the hexagonal 2H  $(3\bar{3}02)$  plane. Experimentally, ribbons of wurtzite silicon [6, 7] and germanium [8] with such an orientation have been produced in a cubic matrix after hardness indentation. The mechanism

of the transformation from the cubic to the hexagonal structure, in terms of dislocations, is analysed accurately in the different papers of Pirouz *et al* [6–8]. Tan *et al* [9] also proposed a model for the formation of hexagonal silicon in ion-implanted silicon wafers. Such a sequence of five- and seven-membered rings is similar to the  $\pi$ -bonded chain model suggested by Pandey for the Si(111)- $2 \times 1$  surface [10]. Odd-membered rings are also found in the ST-12 complex crystal phase of germanium [11]. Moreover, the so-called  $\Sigma 9$  tilt boundary [12], which was studied in the case of two cubic grains of silicon [13, 14], displays the same ring structure.

For both types of interface, we discuss the energetics and the electronic properties, in particular the density of states (DOS) and the band structure. In the case of the (115) interface, the effects of change in ring topology and of non-stoichiometry (presence of Si–Si and C–C bonds) in the boundary regions are discussed.

## 2. Method

Our calculations are based on the density-functional theory (DFT), in the local-density approximation (LDA) [15, 16]. The Vienna *Ab Initio* Simulation Package (VASP) [17] is used. The potential energy of an electron in the field of the nuclei screened by the core electrons is represented by non-norm-conserving ultrasoft pseudopotentials [18]. The single-particle wavefunctions are expanded into a plane-wave basis set. The kinetic-energy cut-off considered is 14.8 Ryd. The electron–electron interaction is described by the Ceperley–Alder functional as parametrized by Perdew and Zunger [19]. The  $k$ -space integrals, which appear in the expressions for the total energy and the electron density, are replaced by sums over special points generated by the Monkhorst–Pack method [20].

The (111) interface is modelled by the supercell represented in figure 2. In each supercell, two interfaces are represented, which are inequivalent due to the presence of two different atoms. The supercell contains 12 pairs of atoms. Six pairs are part of the cubic crystal, six pairs are part of the hexagonal crystal. The lateral lattice constant  $a$  is taken as the value calculated from the elementary cell of the 3C polytype ( $a = 3.055 \text{ \AA}$ ). In the initial geometry, the height of each cubic bilayer is  $2.494 \text{ \AA}$ , the height of each hexagonal bilayer is  $2.501 \text{ \AA}$ . For the mesh of the Brillouin zone (BZ), we use the  $k$ -point grid  $9 \times 9 \times 1$ .

The (115) interface is modelled by the supercell shown in figure 3. The two interfaces represented consist of pairs of rings, one five-membered ring followed by one seven-membered ring, which are periodically repeated along the  $a_1$ -direction. Due to the presence of like-atom bonds in the odd-membered rings, the two interfaces differ from each other too. In the supercell considered, one interface contains three Si–Si bonds, while the other one contains three C–C bonds. The supercell contains 108 pairs of atoms. 56 pairs belong to the cubic crystal, whereas 52 pairs belong to the hexagonal crystal. The structure is arranged in a simple orthorhombic lattice. The lattice vectors are determined from the ideal parameters for  $a$  and for the height of the bilayers, as calculated from the elementary cell of the 3C polytype ( $a = 3.055 \text{ \AA}$ ,  $h = 2.494 \text{ \AA}$ ). The mesh of the BZ considered is  $1 \times 4 \times 1$ .

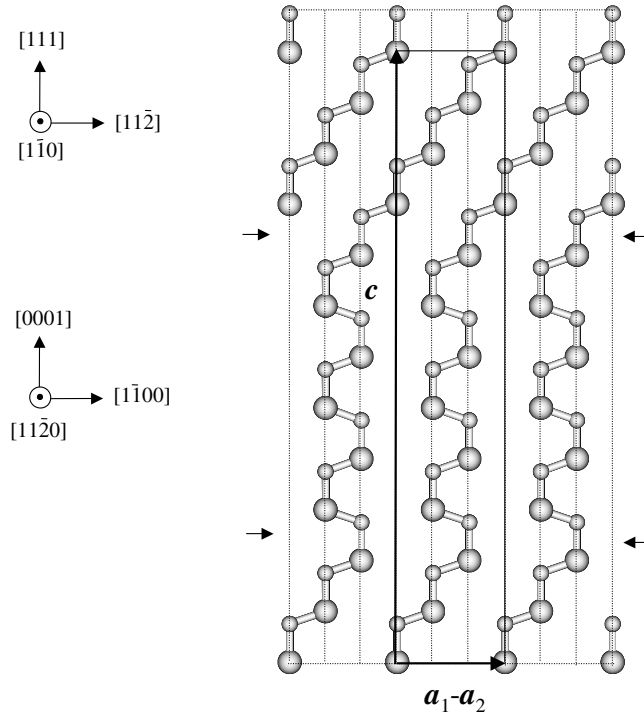
For each supercell, we perform a full optimization of the atomic structure by the minimization of the Hellmann–Feynman forces.

## 3. Results and discussion

### 3.1. (111) interface

The average energy of formation of the interface is calculated according to the formula

$$2E_f = E_{\text{supercell}} - [n_{2\text{H}}E_{2\text{H}} + n_{3\text{C}}E_{3\text{C}}] \quad (1)$$



**Figure 2.** A cross-section of the (111) interface between 3C- and 2H-SiC. The supercell used is represented using full lines, in projection on the (110) plane. The lattice vectors are  $a_1$ ,  $a_2$ ,  $c$ , with  $|a_1| = |a_2| = 3.055 \text{ \AA}$ , and  $|c| = 29.973 \text{ \AA}$ .

where  $n_{2H}$  and  $n_{3C}$  are the numbers of Si–C pairs in the 2H and 3C parts of the supercell, respectively, and  $E_{2H}$  and  $E_{3C}$  are the corresponding pair energies. The calculated energy of formation of one interface per unit area is  $-0.37 \text{ meV \AA}^{-2}$ . The slightly negative value indicates that the creation of such an interface between a cubic and a hexagonal crystal is energetically favoured.

We can also define the energy required to insert a 2H (3C) crystal in a 3C (2H) matrix:

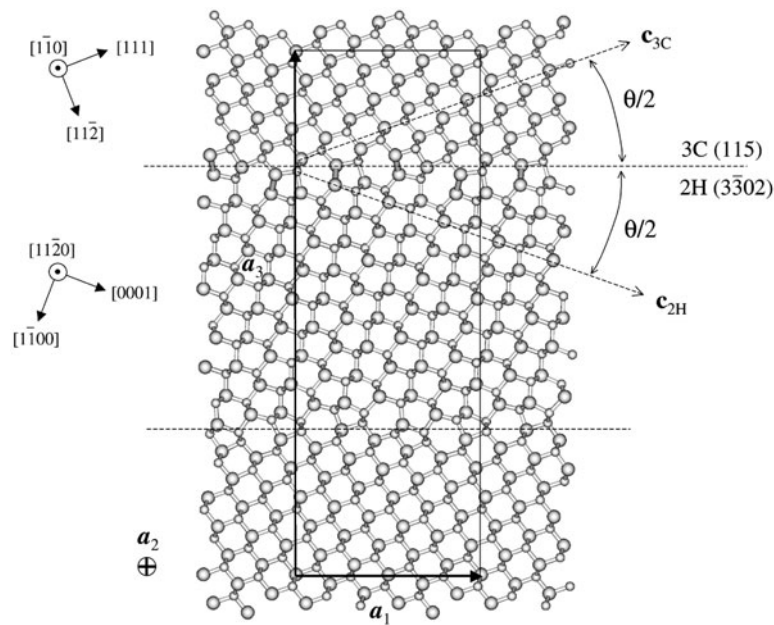
$$E_{\text{insert}(2H)} = E_{\text{supercell}} - nE_{3C} \quad (2)$$

$$E_{\text{insert}(3C)} = E_{\text{supercell}} - nE_{2H} \quad (3)$$

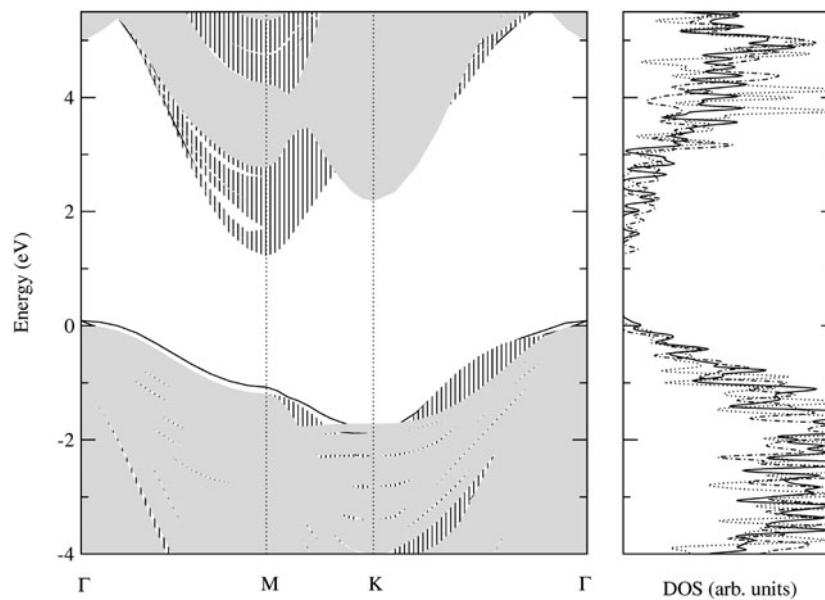
where  $n$  is the total number of Si–C pairs in the supercell. The calculated values are  $E_{\text{insert}(2H)} = 0.66 \text{ meV atom}^{-1}$  and  $E_{\text{insert}(3C)} = -1.16 \text{ meV atom}^{-1}$ . The signs are in agreement with the well-known result that the 2H polytype is less stable than the 3C polytype [21].

The electronic properties are represented in figure 4. The band structure of the interface is shown, together with the projection of the 3C and 2H bulk states onto the interface BZ (hatched and shaded regions). The DOS has also been calculated. The band structure does not indicate any clear interface states in the fundamental gap. Indeed, the band which appears just above the valence-band maximum is too close to the valence-band edge of 2H to be considered as a real interface state, within the accuracy of the calculations.

Another interpretation of the band structures, in terms of stacking faults, can be made. Indeed, if one considers thin 3C layers embedded in a 2H matrix as stacking faults, one can say that such stacking faults induce shallow electronic states in the upper part of the gap of the 2H

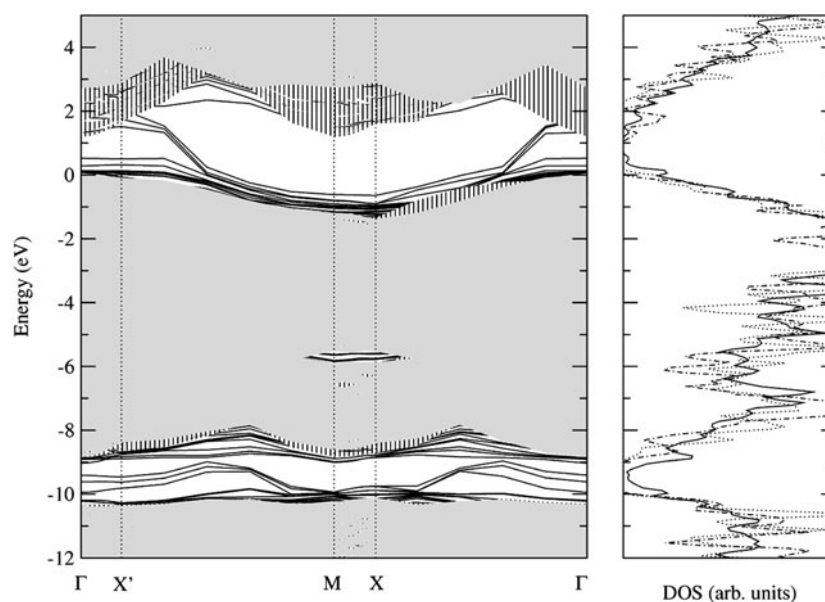


**Figure 3.** A cross-section of the (111) interface between 3C- and 2H-SiC. The supercell used is represented using full lines. The vectors of the simple orthorhombic lattice are  $a_1$ ,  $a_2$ ,  $a_3$ , with  $|a_1| = 15.875 \text{ \AA}$ ,  $|a_2| = 3.055 \text{ \AA}$ , and  $|a_3| = 44.901 \text{ \AA}$ . The tilt angle is  $\theta = 38.94^\circ$ .



**Figure 4.** Electronic structure of the (111) interface. Left: energy bands. The projections of the 3C and 2H bulk bands are hatched and shaded, respectively. Right: the DOS. Solid curve: the structure with an interface; Dot-dashed curve: pure 3C; dotted line: pure 2H.

matrix. As a consequence, stacking faults, i.e. cubically stacked bilayers, in n-type hexagonal polytypes should be electrically active. This is in agreement with the conclusions of Iwata *et al*



**Figure 5.** Electronic structure of the (115) interface. The key is the same as for figure 4.

who found that cubic polytype inclusions in 4H-SiC are efficient traps for conduction-band electrons [22].

### 3.2. (115) interface

The energy of formation of the interface parallel to the (115) plane is found to be positive. The average energy per unit area of one interface is  $0.151 \text{ eV } \text{Å}^{-2}$ . The process of formation of such a complicated interface requires some energy to induce the distortion of the tetrahedra and to generate compressed Si–Si and stretched C–C bonds. The energy for inserting a 2H (3C) crystal in a 3C (2H) matrix with a tilt angle of  $38.94^\circ$  can be calculated as well. Both values are found to be positive and much larger than for the (111) interface ( $E_{\text{insert}(2\text{H})} = 68.4 \text{ meV atom}^{-1}$  and  $E_{\text{insert}(3\text{C})} = 66.9 \text{ meV atom}^{-1}$ ).

The electronic properties are represented in figure 5. In spite of the absence of dangling bonds at the grain boundary, the DOS and the band structure show a lot of interface states within the fundamental and ionic gaps. This results in a metallic behaviour. This can be explained by both chemical and structural effects. These states are generated by the presence of Si–Si and C–C bonds, as well as by the distorted geometry of the odd-membered rings. Indeed, there exist large angular deviations from the perfect tetrahedral angle of  $109.47^\circ$ . The angles vary from about  $90^\circ$  to  $130^\circ$ , which corresponds to deviations of nearly  $\pm 20^\circ$ .

The effects of this special ring topology have been studied in the literature. For silicon and germanium, Joannopoulos and Cohen [23] have shown that odd-membered rings of atoms give rise to states in the pseudo-gap below the bulk valence-band maximum. However, there is a disagreement between Thomson *et al* [14] and DiVincenzo *et al* [13]. Both sets of authors have studied the electronic structure of the  $\Sigma 9$  boundary between two tilted cubic silicon crystals, which also displays five- and seven-membered rings. Only DiVincenzo *et al* find states falling in the bulk band gap. Their DFT-LDA calculations with a local-orbital basis and norm-conserving pseudopotentials predict conduction-band-edge states located in regions of large bond-angle strain.



#### 4. Conclusions

We have examined the electronic properties of two interfaces between 3C- and 2H-SiC. In the case of the (111) interface, the fundamental gap of the projected bulk band structures is almost free of interface states. In contrast, in the case of the (115) interface, the five- and seven-membered rings present together with the Si–Si and C–C bonds generate many interface states in both the fundamental and ionic gaps. As a consequence, we predict that our model of quantum wire constructed from such interfaces will tend to have a metallic behaviour.

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