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2002 J. Phys.: Condens. Matter 14 13031

(http://iopscience.iop.org/0953-8984/14/48/348)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **14** (2002) 13031–13036 PII: S0953-8984(02)54094-7

A molecular dynamics study of the β-SiC/Si(001) interface

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Received 27 September 2002
Published 22 November 2002
Online at stacks.iop.org/JPhysCM/14/13031

Abstract

Despite the large lattice mismatch, SiC is often grown on top of Si substrates. An effective mechanism for accommodating this mismatch is the formation of an array of pure edge dislocations at the interface. We have performed a comparative study of possible core structures of the misfit dislocation via molecular dynamics simulations. We present and discuss the results for the energetics and the structural properties of the most stable configuration.

1. Introduction

Cubic silicon carbide (β-SiC) is an outstanding material due to its unique electronic and structural properties. Its thermal stability, large band gap, high electron mobility and high saturation electron drift velocity suggest it to be a good candidate for applications in high-power, high-frequency and high-temperature devices. Silicon carbide is usually grown on silicon substrates, despite the high lattice mismatch (20%). Recent experiments (Long *et al* 1999) on the characterization of SiC/Si(001) heterostructures by means of high-resolution cross-sectional scanning transmission electron microscopy (STEM) revealed that the interface is locally abrupt and that pure edge misfit dislocations are found, for relaxing the stress induced in the epitaxial layer. However, a microscopic understanding of the atomic structure of the core of such dislocations is still lacking. Furthermore, due to the peculiar value of the misfit in lattice parameters, the SiC/Si system may be considered as a template for the study of edge dislocation arrays at highly mismatched interfaces in compound semiconductors, a topic that still remains largely unexplored.

With the aim of understanding the formation of these self-organized structures, and providing an atomistic description and characterization of the SiC/Si(001) interface, we have

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0953-8984/02/4813031+06$30.00

performed a comparative analysis of possible core structures for the misfit dislocation network using classical molecular dynamics simulations. Among several configurations studied, we found that

(i) a dislocation pinned at the interface is the most stable; and that
(ii) the dislocation core of the lowest-energy configuration shows a deficit in carbon atoms.

2. Method

We performed classical molecular dynamics simulations for the SiC/Si(001) interface, where the Si–Si, Si–C and C–C interactions are modelled by means of the empirical Tersoff potential (Tersoff 1989). Several preliminary calculations have been carried out in order to test the accuracy of these potentials in predicting the structures and relative stability of different Si(001) and β-SiC(001) surface reconstructions, either carbon or silicon terminated. For all the selected test cases we obtained a reasonably good agreement with the reference *ab initio* results (Catellani *et al* 1998). Furthermore, it has recently been found that these potentials give formation energies and properties of native defects in β-SiC(001) in good agreement with DFT *ab initio* calculations (Gao *et al* 2001).

To simulate a realistic system for the SiC/Si(001) heterostructure we considered a slab of material containing up to 60 planes of silicon carbide on top of 60 planes of silicon. For most of the calculations, the interface has been built by matching a p(4 × 4) silicon slab with a p(5 × 5) SiC slab. This corresponds to the introduction of an edge dislocation in silicon carbide every four silicon unit cells, along both the [110] and $[1\bar{1}0]$ directions, as experimentally observed (Long *et al* 1999). A dislocation network is thus generated, originating at the SiC/Si interface, that releases almost all the misfit strain in both directions, perpendicular to the growth axis. We also considered a dislocation array not exactly pinned at the interface, by first inserting one or two pseudomorphic SiC layers between the Si and SiC slabs.

Several interface configurations were considered in our simulations: we studied both C- and Si-terminated interfaces, and under- or over-stoichiometric interface layers. In the calculations, all the atoms in the slab were allowed to move, except the ones in the outermost planes, which were constrained to move collectively only.

In order to compare the interface structures, which may differ in relative number of carbon and silicon atoms, a grand canonical analysis was adopted, following the work of Qian *et al* (1988). In this approach the energy difference between two structures can be written as

$$\Delta E = E_1 - E_2 - \Delta N_{\mathrm{Si}}\,\mu_{\mathrm{Si}} - \Delta N_{\mathrm{C}}\,\mu_{\mathrm{C}} \qquad (1)$$

where E_i is the energy of two selected structures, ΔN_i is the difference in total number of atoms for the ith species and μ_i is its chemical potential. The range of variability of the chemical potential is defined by the limits

$$\mu_{\mathrm{Si(bulk)}} - \Delta H_{\mathrm{f}} \leqslant \mu_{\mathrm{Si}} \leqslant \mu_{\mathrm{Si(bulk)}} \qquad (2)$$

for silicon and

$$\mu_{\mathrm{C(bulk)}} - \Delta H_{\mathrm{f}} \leqslant \mu_{\mathrm{C}} \leqslant \mu_{\mathrm{C(bulk)}} \qquad (3)$$

for carbon; here $\mu_{\mathrm{Si(bulk)}}$ ($\mu_{\mathrm{C(bulk)}}$) is the chemical potential of silicon (carbon) in the stable bulk phase[5] and H_{f} the enthalpy formation energy of bulk β-SiC. Hence, the relation

$$\mu_{\mathrm{SiC}} = \mu_{\mathrm{Si}} + \mu_{\mathrm{C}} \qquad (4)$$

holds, over the full physical range.

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[5] For the carbon species we considered diamond as the stable phase.

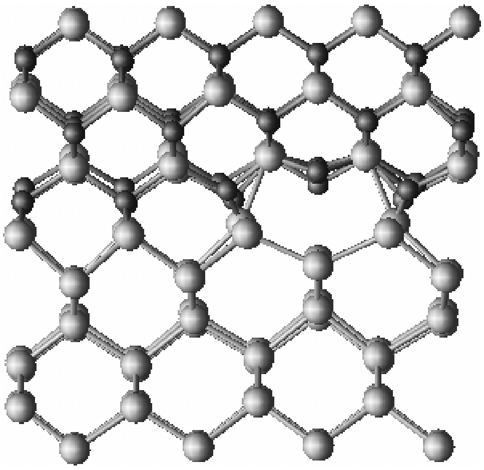

Figure 1. A (110) projection of a stoichiometric SiC/Si(001) interface. Bright (dark) spheres represent silicon (carbon) atoms.

3. Results

When studying the interface system, we first considered the possibility of having heterostructures with β-SiC starting either with a carbon plane or with a silicon one. Our calculations revealed that the interface carbon termination is always favoured. We also found that a pseudomorphic SiC layer on top of silicon before the dislocations start is unfavourable. In agreement with the experimental results (Long *et al* 1999), the most stable configuration is obtained with the dislocations directly pinned at the SiC/Si interface.

The simplest interface structure that we studied, satisfying the conditions mentioned above, is shown in figures 1 and 2, along [110] and $[1\bar{1}0]$ orientations. Here it is relevant to note that the core dislocations in these two perpendicular directions are not equivalent. This is an outcome induced by the peculiar zinc-blende stacking. The interface is stoichiometric with no missing atoms either in silicon or in SiC layers. As can be noted from these figures, the carbon atoms at the core of the misfit dislocation form C–C dimers 1.5–1.6 Å long in order to saturate their dangling bonds. We also observed that both Si–Si (in Si) and Si–C bonds (in SiC and at the SiC/Si interface) are stretched close to the interface, compared to the bulk bond lengths of the host materials, being respectively elongated to 2.5 and 2.0 Å. The tetrahedral configuration is distorted, too, with some of the Si–C–Si bond angles up to 123°. The bulk structure is quickly recovered when moving away from the interface and at the fourth atomic layer the residual distortions have already become small ($\pm 1.5\%$ in bond distances and $\pm 5\%$ in bond angles).

Different metastable structures are obtained from the previous one by removing carbon atoms from the dislocation cores. In particular, the most stable configuration is obtained when removing the extra line of carbon atoms present at the stoichiometric interface in the [110] direction (compare figures 1 and 3) and the entire row of carbon dimers in the $[1\bar{1}0]$ direction (compare figures 2 and 4): indeed, no dangling bonds are present in this system.

The energy gain found going from the optimal stoichiometric interface to the most stable one is -0.48 J m^{-2} for C-rich growth conditions and -1.12 J m^{-2} for C-poor conditions. The two dislocation cores are again non-equivalent in the two directions represented in figures 3 and 4 and a distortion in bond lengths and bond angles similar to that in the stoichiometric case is observed. Further removal of carbon atoms from the interface is unfavourable. This seems

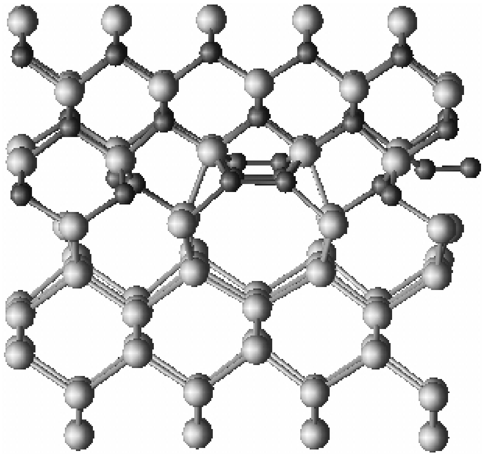

Figure 2. A ($1\bar{1}0$) projection of a stoichiometric SiC/Si(001) interface. Bright (dark) spheres represent silicon (carbon) atoms.

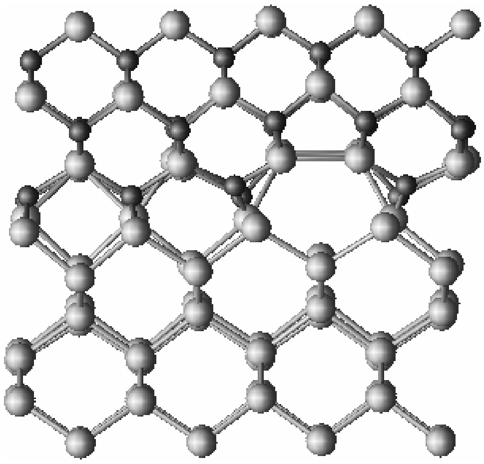

Figure 3. A (110) projection of the most stable SiC/Si(001) interface. Bright (dark) spheres represent silicon (carbon) atoms.

to indicate a competition between two opposite tendencies, connected with the presence of carbon at the interface: the chemical energy gain due to the SiC bond formation at the interface and the strain energy gain associated with the removal of C atoms from the dislocation core. Reasonably, the minimum structure that we found is the one that realizes the best compromise between these two contributions.

We finally considered the possibility of having extra carbon atoms at the SiC/Si interface, putting on top of the silicon substrate an over-stoichiometric SiC layer (carbonized interface layer). We always found structures higher in energy than the stoichiometric one, for the full physical range of chemical potentials.

As discussed above, large slabs were adopted in this work, up to 120 layers: this choice allows us to get an estimate of the elastic contribution to the total energy of the system, which can be expressed within the elasticity theory, following, e.g., Bonnet (Bonnet and Verger-

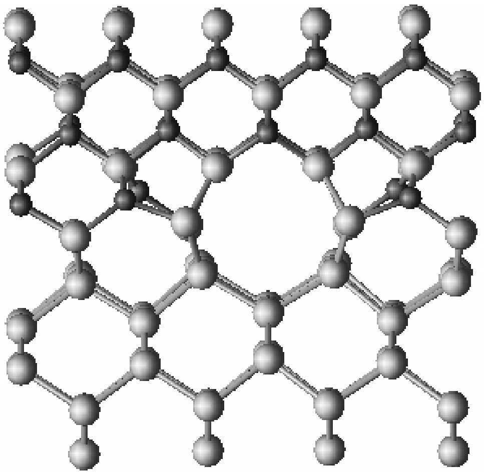

Figure 4. A $(1\bar{1}0)$ projection of the most stable SiC/Si(001) interface. Bright (dark) spheres represent silicon (carbon) atoms.

Gaugry 1992). The calculated defect energy can be written as

$$E_{\mathrm{D}} = E_{\mathrm{interface}} + E_{\mathrm{interface-surface}} \tag{5}$$

$$E_{\mathrm{D}} = E_{\mathrm{elastic}} + E_{\mathrm{non-elastic}} + E_{\mathrm{interface-surface}}. \tag{6}$$

Here E_{D} is the defect formation energy: this can be considered as the sum of different contributions: the interface part as itself ($E_{\mathrm{interface}}$) plus the interface-to-surface interaction ($E_{\mathrm{interface-surface}}$). Furthermore, $E_{\mathrm{interface}}$ may be regarded as the sum of the elastic (E_{elastic}) and inelastic terms ($E_{\mathrm{inelastic}}$). When the number of planes of the slab is large enough, $E_{\mathrm{interface-surface}}$ is vanishing. If all the defect energy is considered as elastic, the calculated edge dislocation core radius is 3.186 Å in C-rich conditions, for the most stable configuration. The large value obtained in the present calculations, with respect e.g. to a Burgers vector of $\simeq$3.072 Å, for edge dislocations in SiC, is due to interface effects. The defect energy of the dislocation network for this structure is estimated to be 0.11 J m^{-2} in C-rich and 0.75 J m^{-2} in C-poor conditions, within elasticity theory (Bonnet and Verger-Gaugry 1992). The large lattice mismatch between the two materials and the difference in elastic constants account for these numbers.

4. Conclusions

In conclusion, we have studied and characterized the structure and the stoichiometry of the SiC/Si(001) interface. We found that it is favourable to have C atoms at the interface and that the edge dislocations, needed to minimize the extreme lattice mismatch between the two materials, are directly pinned at the interface, in agreement with experimental observations (Long *et al* 1999).

Furthermore, under-stoichiometric interfaces are always more stable than stoichiometric or over-stoichiometric ones. A detailed description of the structural and electronic properties of these mismatched interfaces requires *ab initio* simulations (Cicero *et al* 2002).

Acknowledgments

This work was partially supported by INFM-PRA:1MESS; computing facilities in CSCS, Manno (CH), are gratefully acknowledged.

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