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Ab initio calculation of the structural and electronic properties of the SiC (100) Surfaces

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Abstract

In this work, we have calculated ab initio the structural and electronic properties of both the C- and Si-terminated SiC (100) surfaces in the c(2×2) and (2×1) reconstruction patterns, respectively. Based on our results, we found that the Si-terminated surfaces is dominated by weak bonded Si-dimers, which is stabilized only at Si-rich conditions, leading to a (3×2) or more complex reconstruction patterns, as verified experimentally. Also, our results show that the C-terminated surfaces is characterized by strong triply-bonded C-dimers, in a c(2×2) reconstruction pattern, which consists of C_2 pairs over Si bridge sites, which is consistent with the experimental results.

Keywords: Surfaces; Total energy; Reconstructions; Silicon carbide

1. Introduction

SiC is the most indicated material for the high temperature semiconductor devices, besides the fact that this compound is the most promising substrate for the epitaxial growth of III-Nitrides [1,2]. For this specific growth, the most common substrate surface used is the (100) one, and there has been a great interest for the understanding their structural and electronic properties.

It is well known that (100) surfaces are formed by arrangements of dimers, leading to reconstructions of a large degree of multiplicity and complexity [3]. In the case of SiC, while the Si-terminated surfaces are stable within the (5×2), c(4×2), (3×2) or (2×1) reconstruction patterns at Si-rich conditions, the C-terminated ones, which is known by its chemical inertness and thermal stability, are characterized by an interesting c(2×2) arrangement of C-dimers, each one consisting with a double or a triple bond among the C atoms, which were described by two competing models: the Bridge-Dimer Model (BDM) and the Staggered-Dimer model (SDM) [4,5].

In order to understand, the complexity of the reconstructions of SiC surfaces, we present in this work, a preliminary comparative study of the geometry, bond behaviour, the energetics as well as the electronic structure for the (2×1) reconstruction model of the Si-terminated surfaces, and for (2×1) and c(2×2) reconstruction patterns within both BDM and SDM models of the C-terminated ones. Our results were obtained ab initio by using the Density Functional Theory within the Local Density Approximation, plane-wave description of the wavefunctions and the pseudopotential method (abinit code) [6], together with the slab-supercell description of the surfaces. We have used the Troullier–Martins pseudopotentials (fhi98PP code) [7], following the recipe developed by Stampfl and Van de Walle [8]. The C(Si)-terminated surfaces were described by slab supercells build up of 6(5) atomic layers and a vacuum region equivalent of 4(5) atomic layers, and the back surface was passivated by hydrogen atoms. For the slab lattice parameters, we have used our calculated equilibrium bulk lattice parameter for cubic SiC, 4.31 Å, obtained with a cutoff energy of 35 H (70 Ry) for the planewaves and 10 special **k**-points. Also, in the slab calculations, a (4 4 2) Monkhorst–Pack set of **k**-points was used to sample the slab Brillouin zone [9], and we kept the same cutoff energy for the plane-waves.

2. C-terminated surfaces

It is well known that, for the C-terminated surfaces, there are two competing models that explain the observed c(2×2)

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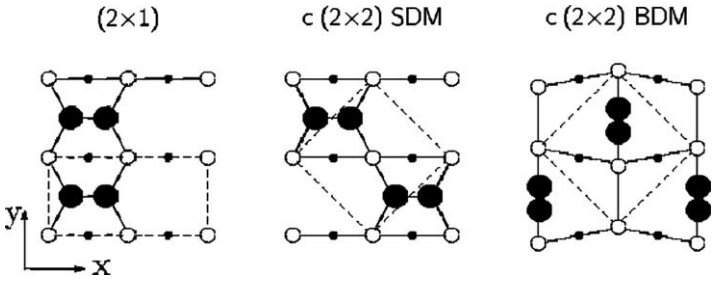

Fig. 1. Top view of the accepted models for the (2×1) and c(2×2) reconstruction models of the C-terminated SiC (100) surfaces.

reconstruction, the BDM and the SDM, which is directly related to the two possible preparation methods for this surface [5]. These two models are depicted in Fig. 1, together with the (2×1) reconstruction pattern. In Table 1, we display the structural parameters for the reconstructed surfaces as defined in Fig. 2, and we have verified that our results are in good agreement with other previous theoretical and experimental results [4,5].

From Table 1, we checked that both bond angles, α and β, tend to 120°, indicating that each C-dimer atom tries to make planar bonds with the other one. Also, it is interesting to note that, in both the (2×1) and the SDM patterns, the surface moves inward, while in the BDM, the surface relaxes in the opposite way. This is a clear indication that the C–C bonds, in the latter model, have different character when compared with the previous one. Moreover, if we look at the dimer bond length (parameter A), in both the (2×1) and the SDM it approaches to the C–C double bond, as verified for the ethylene, while in the BDM, it is close to the C–C triple bond of the acetylene. So, our results are in consonance with previous total energy calculations [5,10], and also, confirms that the C-terminated surface is completely dependent of its preparation method.

It is also interesting to note, from Table 1, that there is a Si-dimer at the sub-surface in the BDM, once the value for the parameter D is 2.39 Å, and this is a fingerprint of this specific model.

From the total energy point of view, the BDM is 7.0 meV/atom more stable than SDM, in agreement with the results of Käckell et al. [10]. However, the BDM is only favored by 2 meV/atom over the (2×1) reconstruction pattern. Based on the fact that our calculations have the accuracy of 0.2 meV/atom, and that the total energy differences between these three models are small, we can deduce that these patterns can coexist at high temperatures.

When we look at the calculated electronic band structures of these models, our results show that while for the (2×1) pattern, it has a metallic character, for both the BDM and SDM they have a semiconductor character instead. In Fig. 3, we depicted the calculated electronic band structure for the BDM.

From Fig. 3, we found that, at Γ point of the Brillouin zone, there are two states in the bandgap, one at $E_c+0.84$ eV, and the other at $E_c+0.50$ eV, both fully occupied. While the first one has the main contribution from the Si sub-surface atom, remaining in the gap with a small dispersion of 0.67 eV, the second one has a strong C-dimer π-bond character, as that observed on the C–C triple bonds in the acetylene molecule. The latter has a strong dispersion, of around 1.5 eV, so that it leaves the gap at the M point. Also, the first unoccupied level, which is resonant at the conduction band at $E_c+3.58$ eV in Γ, has a π antibonding character, and a flat dispersion, lying in the bandgap at the M point.

We would like to mention that the calculated band structure of the SDM has almost the same appearance of that of BDM: there are three occupied levels in the bandgap with the highest occupied level located at $E_c+0.84$ eV having the same character of the highest occupied level of BDM, and the lowest unoccupied, $E_c+2.41$ eV, is also resonant at the conduction band, but has 1.0 eV of dispersion and has the same features of the C–C double bonds in the ethylene molecule.

Table 1
Calculated structural parameters, as defined in Fig. 2, for the C-terminated SiC (100) surfaces in the p(2×1), c(2×2)SDM and c(2×2)BDM reconstruction patterns depicted in Fig. 1

Model	α (degrees)	β (degrees)	z (Å)	A (Å)	A_{exp} (Å)[5]	B (Å)	C (Å)	D(Å)
p(2×1)	112.02	110.77	−0.29	1.43	1.31	1.84	3.05	2.73
c(2×2) SDM	105.64	115.94	−0.20	1.37	1.31	1.91	3.05	3.05
c(2×2) BDM	–	133.00	0.21	1.23	1.22	1.82	3.12	2.39(2.70)[a]

The datum in the parenthesis of the last column is the experimental result for the Si-dimer in the BDM, taken from Ref. [5].
[a] There is a Si-dimer at the sub-surface, which is a fingerprint of this specific model [4,5].