# Atomic structure of β-SiC(100) surfaces: an ab initio study

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## Abstract

We examine several different reconstructions of the β-SiC(100) surface by the ab initio Car–Parrinello method. Our results confirm that the lowest energy c(2 × 2) reconstructed surface consists of triply bonded carbon dimers in a bridging position between neighboring underlying silicon dimers. Added hydrogen atoms bond to the carbon dimers, resulting in a lengthened double-bonded dimer, and a larger separation for the underlying silicon dimers, although those Si bonds do not disappear. The most stable structure found for the (3 × 2) reconstructed surface with a 1/3 monolayer excess of silicon is an alternate dimer row structure rather than the added dimer row model proposed by others. The energetics of various surface reactions that may be involved in growth of SiC are discussed.

## 1. Introduction

Silicon carbide, SiC, is a wide band-gap (2.2 eV) semiconductor with several outstanding properties, such as high thermal stability, high electron mobility and high thermal conductivity, giving it a tremendous application potential in high-temperature, high-frequency and high-power electronic devices [1]. This has spurred a great deal of effort in characterizing its properties and in finding ways to grow high-quality crystals. In particular, much attention has been focused on the surface atomic structure of the cubic polytrope, β-SiC or 3C-SiC. The technology for depositing a high-quality crystalline film over a large area is needed in order to make use of SiC in device

fabrication. Knowledge of the atomic and electronic structure of SiC surfaces is essential for understanding and controlling surface processes in film growth.

Several studies of SiC chemical vapor deposition have used alternating exposure of the surface to disilane, $Si_2H_6$, and acetylene, $C_2H_2$, or ethylene, $C_2H_4$, in a temperature range of 850–1050° C to grow the (100) face of β-SiC [2–4]. In this orientation the crystal corresponds to alternating layers of Si and C. The growth is "self limiting" in this temperature range, i.e. after prolonged exposure to only one of the two chemicals the surface becomes nonreactive and growth terminates. While the Si-terminated (100) surface of a SiC crystal has (2 × 1) symmetry, analogous to the (100) surface of pure Si and diamond [5], the surface obtained after long-time exposure of SiC to $Si_2H_6$ has (3 × 2) symmetry. This structure has been determined to correspond to a Si-enriched surface with an additional coverage of

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Si corresponding to 1/3 of a monolayer beyond a Si layer in a SiC crystal. A shorter exposure to $Si_2H_6$ can produce a surface with $(5 \times 2)$ symmetry and this has been found to correspond to an extra Si coverage of 1/5 of a monolayer [6,7]. On the other hand, prolonged exposure to $C_2H_2$ results in a surface corresponding to one monolayer of C. Unlike the (100) surfaces of Si and diamond, the symmetry of the C-terminated SiC surface is $c(2 \times 2)$ [2,3]. The growth sequence is reversible and can be summarized as

$$c(2 \times 2) \leftrightarrow (2 \times 1) \leftrightarrow (5 \times 2) \leftrightarrow (3 \times 2), \qquad (1)$$
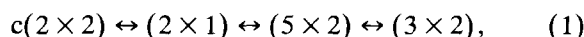
where exposure to $Si_2H_6$ changes the surface structure stepwise in the order from left to right, but exposure to $C_2H_2$ changes the surface structure in the opposite direction [3]. Long-time annealing of the Si-terminated SiC surfaces in vacuum at 1250° C also results in the formation of this carbon-terminated $c(2 \times 2)$ surface [8].

While the $(2 \times 1)$ surface structure is clearly analogous to the well known dimer structure of the Si(100) and C(100) surfaces, the atomic configurations corresponding to the other reconstruction patterns are quite unique and not well understood. In particular, controversy remains about the structure of the C-terminated $c(2 \times 2)$ surface. Contradictory conclusions have been reported as a result of separate experimental studies [8,9] as well as from separate theoretical studies based on semi-empirical calculations [10,11]. Even less is known about the $(3 \times 2)$ surface. Models have been proposed [6] based solely on the coverage data but no experimental or ab initio studies of the atomic structure have been reported. Optimization of crystal growth by atomic level control of the growth processes clearly requires better knowledge of the atomic structure of these surfaces.

One issue, for example, is the fate of the extra 1/3 monolayer of Si present on the $(3 \times 2)$ surface when exposed to $C_2H_2$ or $C_2H_4$. Some groups have advocated precise control of the $Si_2H_6$ supply to form only the $(2 \times 1)$ structure in order to realize single monolayer growth of SiC [4], and argued that the additional Si in the $(3 \times 2)$ surface results in a non-stoichiometric Si-rich film. Others have suggested that the extra Si desorbs during $C_2H_2$ exposure and that one monolayer of SiC is deposited

epitaxially per growth cycle [2]. Still others claim that any additional Si present on the surface is incorporated in the SiC crystal and contributes to increased crystal growth [3]. Our calculations cannot settle this question since we have not been able to examine the associated barriers, but we do find that all of these possibilities are energetically plausible and it is possible that each process may occur, depending on the growth environment.

## 2. Calculations

We report here results of a study of the atomic and electronic structure of $c(2 \times 2)$ and $(3 \times 2)$ surfaces using ab initio density functional theory (DFT) calculations in the Car–Parrinello scheme [12]. We use norm-conserving non-local pseudopotentials [13,14] and a plane-wave basis set for the electronic states. An energy cut-off of 40 Ry for the plane-wave expansion was used. In the calculations of $c(2 \times 2)$ surfaces, we have used a unit cell of 8 layers with 8 atoms per layer. The bottom four layers are frozen in their bulk positions and there is an 8.5 Å vacuum spacing above the surface. For the $(3 \times 2)$ surface, a similar unit cell of 8 atomic layers was used with 6 atoms per layer, plus a Si ad-dimer on the top surface, representing a 1/3 excess coverage of silicon. We have previously reported [15] on studies of these same surfaces using the empirical potential of Tersoff [16] and discuss below how they compare with the ab initio results.

The initial atomic configurations used in the DFT calculations were generated using the Tersoff potential. The electronic and ionic degrees of freedom were then relaxed simultaneously using a parallel implementation of the Car–Parrinello method [17]. Our calculations of the bulk properties of cubic SiC provide a lattice constant of 4.29 Å, which is 1.6% below the experimental value of 4.36 Å. The bulk modulus is calculated to be 2.37 mbar which compares well with the experimental value of 2.24 mbar. The calculated cohesive energies are about 33% too large in the local density approximation (LDA) and 24% too large with the Perdew–Wang'91 (PW91) gradient correction [18], but this may be attributed to the inadequacy of these density functionals in de-

scribing the isolated (pseudo-)atom, which is needed for calculation of a binding energy. In this study we rely on relative energies rather than their absolute values. We also performed a calculation on the free C–C dimer to test the validity of the pseudopotential in structures with very short bond length. The equilibrium bond distance was calculated to be 1.24 Å in excellent agreement with the experimental value of 1.243 Å [19] and with high-level configuration –interaction calculations [20]. Calculations of acetylene, $C_2H_2$, ethylene, $C_2H_4$, and ethane, $C_2H_6$, also gave correct bond lengths within 0.015 Å of experiment and structures with the correct symmetry (the bond angles differed from experimental values by less than 1 degree). The C–C bond lengths are calculated to be 1.193 Å in acetylene (a triple bond), 1.315 Å in ethylene (a double bond), and 1.524 Å in ethane (a single bond). We also evaluated a bonding parameter obtained by averaging the charge in a cylinder centered on the middle of the C–C bond. The resulting numbers of 0.155, 0.109 and 0.067 electrons/$a_0^3$ for acetylene, ethylene and ethane, respectively, can then be used in a comparative manner to determine the bond character of the C–C bonds we study.

We also supplement these LDA calculations with a calculation of gradient corrections to the total energy. In particular, we report binding energies using the Perdew–Wang (1991) formulation [18]. The energy values discussed below include this contribution unless otherwise specified. Both sets of results are shown in Table 1. There was little difference between relative energies in the LDA and with the PW'91 corrections. The total energies obtained in these slab calculations are reported as surface ener-

Table 1
Surface energies above the bulk for the various reconstructed surfaces, in eV per (1 × 1) surface cell

|                             | LDA  | PW'91 |
|-----------------------------|------|-------|
| Si(1 × 1) unreconstructed   | 2.69 | 2.74  |
| C(1 × 1) unreconstructed    | 2.91 | 2.70  |
| Si(2 × 1) relaxed           | 2.24 | 2.29  |
| c(2 × 2) surfaces           |      |       |
| C pair on bridge            | 1.25 | 0.89  |
| Staggered C dimer           | 1.42 | 1.23  |
| (3 × 2) surfaces            |      |       |
| Alternate dimer row         | 1.54 | 1.62  |
| Added dimer row             | 2.17 | 2.21  |

gies in Table 1. We have used an even number of atomic layers as far as possible in order to make comparison with bulk energies more direct. This means that the two free surfaces consist of opposite species (either Si or C), and the one not being studied is frozen in the bulk (unrelaxed (1 × 1) surface) geometry. The surface energies for the unrelaxed (1 × 1) surfaces were evaluated by allocating the bulk binding energy (relative to the atomic energies of Si and C) equally between Si and C atoms, and by carrying out one run with an odd number of layers to extract the energy for a Si(1 × 1) surface alone. This procedure may introduce errors in the absolute surface energies reported in Table 1, but relative surface energies of different structural models for the same surface are not affected since the number of atoms is the same.

## 3. Results

Our calculation of the Si-terminated $\beta$-SiC(100) used a starting configuration with rows of symmetric dimers and a (2 × 1) structure but the final, relaxed structure had p(2 × 2) symmetry as the dimers tilt in a staggered pattern. The relaxation energy given by the difference of the total energy with respect to that of an unrelaxed (1 × 1) surface is 0.90 eV per surface dimer. This can be compared with 1.01 eV obtained using the Tersoff potential [15]. The dimer bond length is 2.26 Å and the height difference of the Si atoms in the tilted dimer is 0.05 Å. These values agree reasonably well with a dynamical LEED study by Powers et al. [21] who determined 2.31 and 0.2 Å, respectively. This dimer bond length is substantially shorter than that found on pure Si(100)-(2 × 1) surfaces, where the distances are 2.47 and 0.36 Å, respectively [22]. We note that p(2 × 2) is not an experimentally observed symmetry and is likely due to the size and shape of the unit cell used in our calculation. The energy associated with the tilt is small, significantly less than 0.1 eV per dimer and the energy difference between different patterns of the tilted dimers is even smaller. A different pattern for the tilting of the dimers can result in the c(4 × 2) symmetry which is sometimes observed experimentally, but simulation of the c(4 × 2) configuration would require a larger simulation cell than we have

used. The tilting of Si dimers and various structural patterns that can result from that have been studied extensively for Si(100) surfaces [23].

### 3.1. The c(2 × 2) surface

The carbon-covered c(2 × 2) surface has stimulated much interest and controversy. One of two competing models was proposed by Bermudez and Kaplan [8]. It is qualitatively similar to the dimer model used for the (2 × 1) surfaces except that the c(2 × 2) symmetry results from a staggered arrangement of the dimers instead of dimer rows as illustrated in Fig. 1a. Their model is based on several measurements, including AES, ELS and LEED. In particular, they conclude that the surface has C

dangling bonds which can be saturated by H adsorption. This model has received support from a semi-empirical calculation by Craig and Smith [10] using the SLAB-MINDO method. However, the calculated results indicate that the surface carbon dimer has a double bond and no dangling bond. An alternative model was proposed by Powers et al. [9] based on dynamical LEED analysis. It is qualitatively very different from the dimer structures which apply to the Si-terminated SiC(100) surface and the (100) surfaces of pure Si and C. The proposed structure is illustrated in Fig. 1b. A carbon dimer is placed in bridge sites formed by a staggered array of Si dimers in the second layer. This model has received support from the MNDO calculation of Badziag [11].

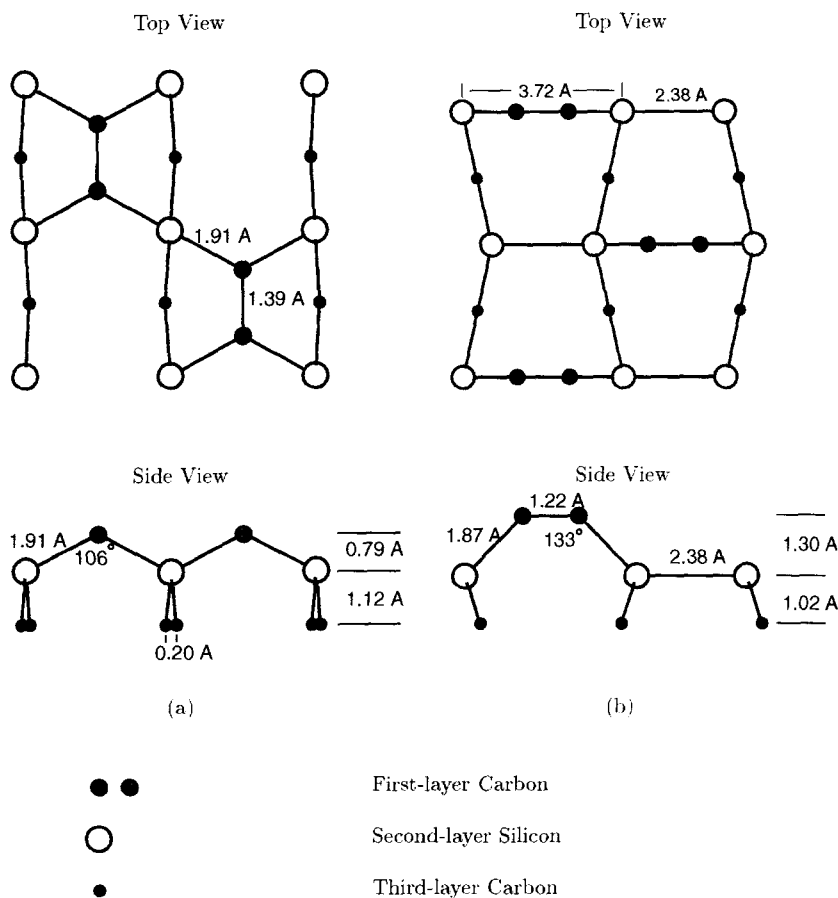The results of our calculations of these models,



Fig. 1. Models for the C-terminated c(2 × 2) surface: (a) staggered C-dimer structure, c(2 × 2)ₐ; (b) C-dimers on top of Si bridge sites, c(2 × 2)ᵦ. The structural parameters are obtained from our calculations.

including the LDA results and gradient-corrected results, are listed in Table 1. Both reconstructions significantly lower the energy (by 3.0 to 3.6 eV per C pair) from the ideal (1 × 1) carbon-covered surface, but the model of Powers et al. with carbon pairs in the Si bridge sites is favored energetically over the staggered carbon dimer model by 0.68 eV per surface C pair in the PW91 results.

Fig. 1 gives the structural parameters of the LDA-relaxed configuration for these two models. In the staggered carbon dimer model, in Fig. 1a, the dimer bond length is 1.39 Å, consistent with a double bond. The Si–C bond length on the surface is 1.91 Å relative to 1.87 Å in the bulk. The surface carbon dimers have very little tilt and the underlying Si layer is *not* dimerized but has a slight 0.03 Å
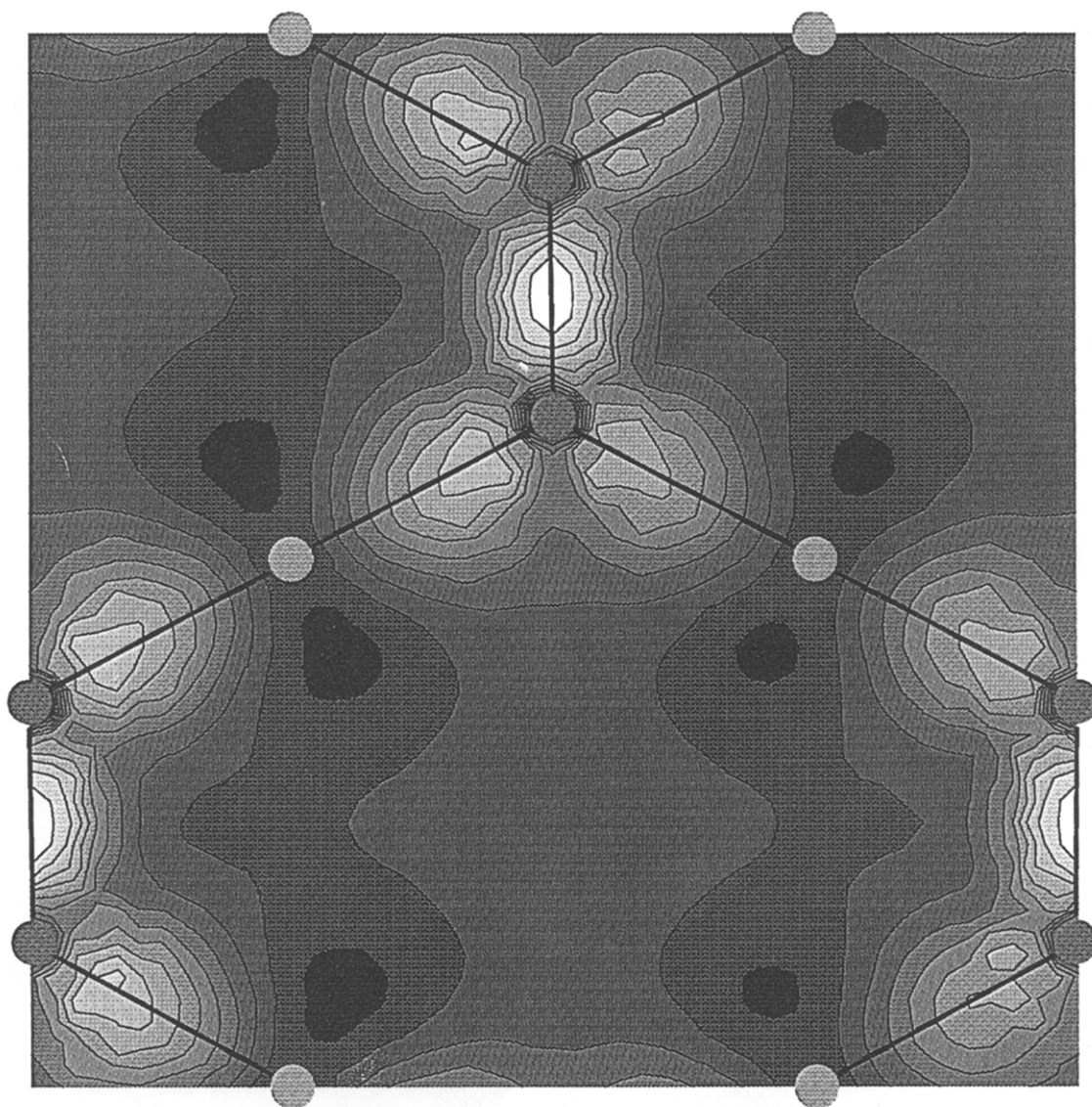


Fig. 2. Contour plot of the charge density differential sliced across surface C dimers for the staggered dimer model of the c(2 × 2) surface. The darker circles are the C atoms, the lighter circles are the Si atoms in the layer below.

buckling. The distances between layers 1 and 2 and between layers 2 and 3 are 0.79 and 1.12 Å, respectively. The resulting structure generally agrees quite well with the results of Craig and Smith [10] for this model. Fig. 2 shows contour plots of the charge density differential sliced across a surface dimer. It demonstrates clearly the $>C-C<$ bonding arrangement with the indication that the C–C bond may be a double bond. This can be seen from the intensity of the contour shades in Fig. 2.

For the model of Powers et al. with bridging C pairs, shown in Fig. 1b, the bond length in the C pair is 1.22 Å, and the Si–C bond length is 1.87 Å, indicating much stronger bonding on the surface. The sublayer Si atoms are, furthermore, dimerized in our calculation, with a dimer length of 2.38 Å. This
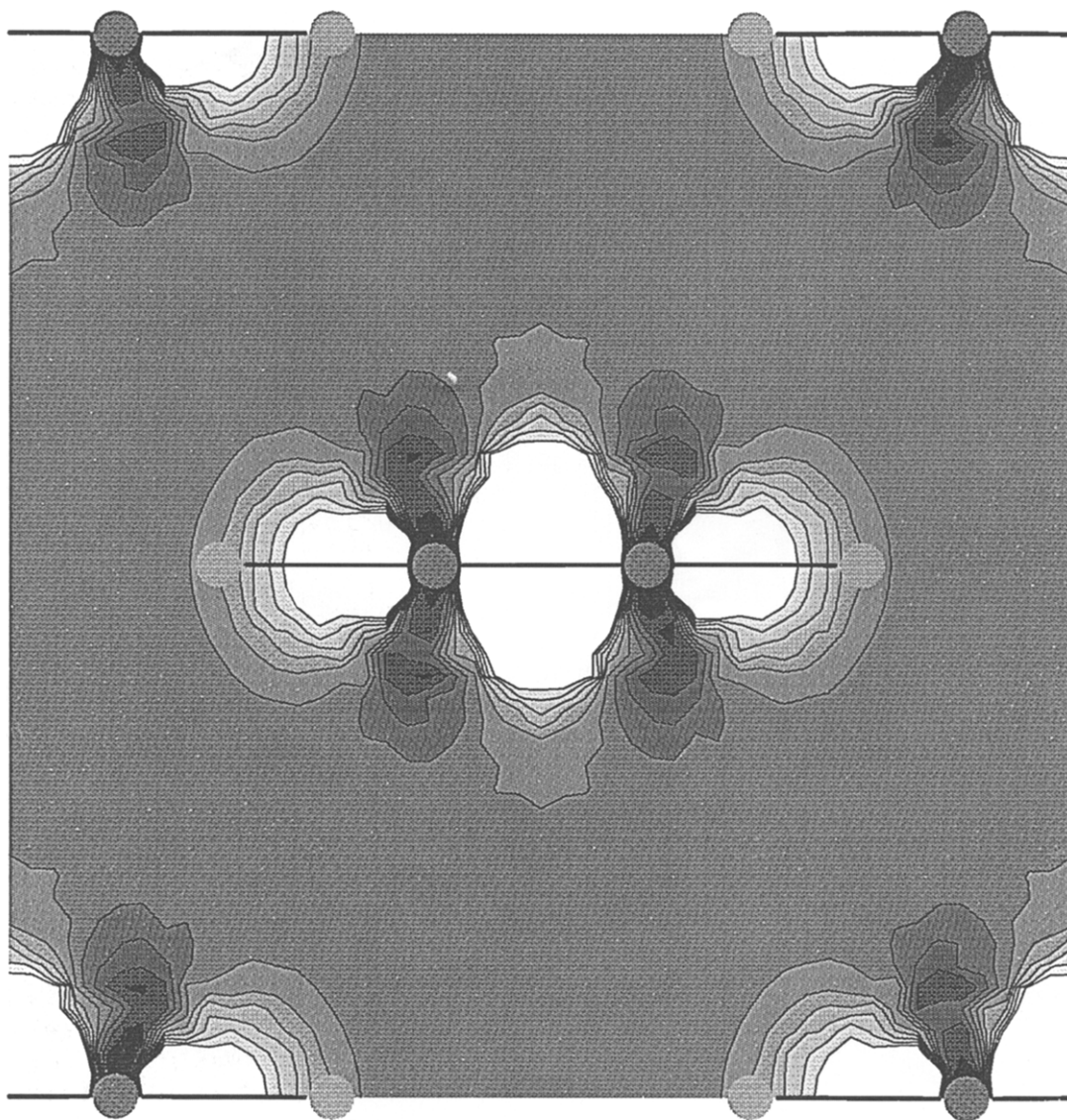


Fig. 3. Contour plot of the charge density differential sliced across surface C pairs for the model with the C pairs in the Si bridge sites of the c(2 × 2) surface.

agrees with the results of Badziag [11] (who found a C–C pair distance of 1.21 Å and a Si dimer length of 2.55 Å). The sublayer dimerization was not observed in all the LEED experiments [9], however: samples obtained by Si evaporation did show dimerization, while samples prepared by adsorption of $C_2H_4$ did not, but this may be related to the expansion of the sublayer dimer bonds we see upon hydrogenation of the surface (see below). We have calculated the energy required to destroy the underlying Si dimers in this system and found it to be very large, 1.84 eV/dimer. It may be the lack of Si dimerization in the staggered dimer model that makes it unfavorable relative to this bridge pair model. The C–C distance in the surface carbon pair is indicative of a triple bond. To confirm this, we also evaluated the bonding parameter discussed earlier. The value of this param-

eter was 0.143 for the C–C bond in the bridge model, close to the value for acetylene, indicating that the bridge C–C bond is indeed close to being a triple bond.

Charge density differential contour plots sliced across the surface carbon pairs are shown in Fig. 3. These indicate the very strong bonding between the carbon pairs, and the absence of dangling bonds on the surface. Because we use a plane-wave basis set there is not an easy way to assign charge to the individual atoms in our calculation. Examination of the layer-by-layer-integrated charge density indicates that the surface C atoms in the bridge model for the $c(2 \times 2)$ surface are significantly closer to neutral charge than the bulk atoms in SiC, which have been established by other methods to gain on average 0.6 electrons lost by the silicon. By contrast, in the
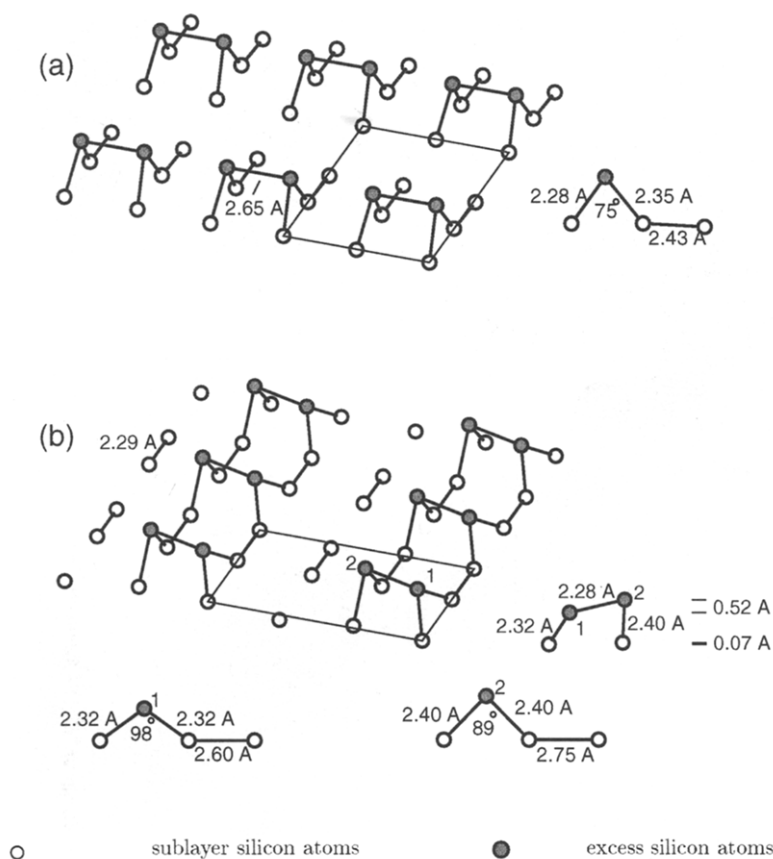


Fig. 4. Models for the $(3 \times 2)$ surface with extra 1/3 monolayer of Si atoms on top of a silicon layer: (a) added dimer row model; (b) alternate dimer row model proposed here.

staggered dimer model the charge on the surface carbon atoms seems to be almost identical with that in the bulk.

Our earlier calculations [15] with the Tersoff potential favored the staggered dimer reconstruction over the bridging structure in disagreement with the density functional calculations. We find two possible causes for this failure: first the Tersoff potential is not designed to deal with the short bond lengths associated with triply bonded carbon, and therefore
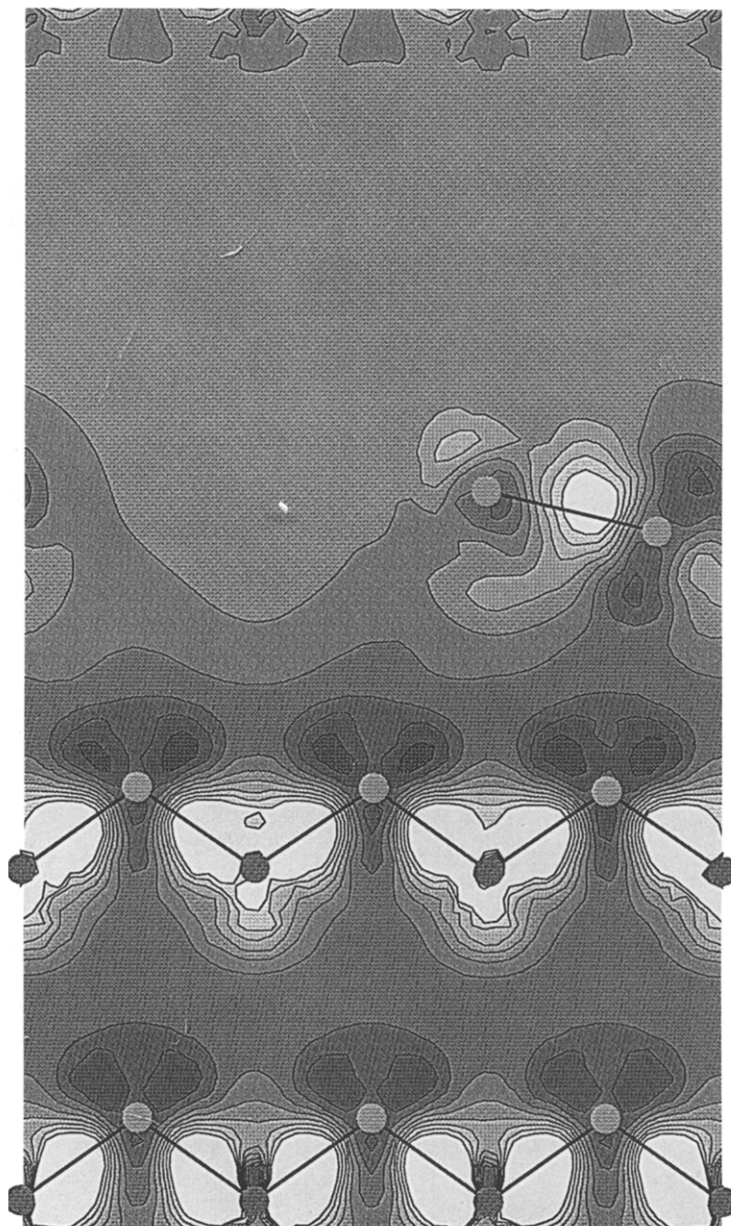


Fig. 5. Contour plot of the charge density differential in a vertical slice for the (3 × 2) surface in the alternate dimer model proposed here. The dark and light atoms are again C and Si, although all the atoms drawn are located in the plane (there are intervening C and Si layers not in this plane). Note the extra charge on the upper Si of the ad-dimer.

gives the bridged structure a double or single bond, and a consequently higher energy. Second, the charge transfer variation mentioned in the preceding paragraph means that the surface charge distribution is quite different from the bulk and also differs between the bridged and staggered dimer configurations, and any empirical potential (like the Tersoff potential) will be unable to account for this change in relative charge on the atoms.

It is possible that hydrogen may be present on the surface for most growth conditions for the c(2 × 2) surface. We have tested several sites and found that the only location where hydrogen atoms will bind is to either end of the surface carbon dimers. This released 2.30 eV for each deposited $H_2$ molecule. This is significantly larger than the 1.55 eV found by Badziag [11] and would result in a significantly greater level of hydrogenation of the surface under typical experimental situations. The resulting surface with maximal hydrogen concentration (essentially $C_2H_2$ added to a dimerized Si surface) has the carbon–carbon dimer distance increased to 1.34 Å, close to the length of a typical C–C double bond and the averaged charge density in the cylinder containing the middle half of the C–C bond is 0.100 compared with 0.109 for the C–C bond in ethylene. The Si–C bond length has increased to 1.90 Å and the Si–Si dimer bond length has increased to 2.52 Å. Badziag found a similar increase in bond lengths on adding hydrogen, with 1.33 Å for the C–C length and 2.70 Å for the Si–Si dimer.

Attempts to hydrogenate the Si dimers in the second layer led to spontaneous desorption and regeneration of the dimers as the structure was relaxed.

## 4. The (3 × 2) surface

Based on experimental measurements [6,7], indicating that the excess Si coverage is 1/3 monolayer on the (3 × 2) surface, Hara et al. have postulated an added dimer row model [6], in which dimers are formed in the top layer in the direction perpendicular to that of the sublayer dimers. Although this model, illustrated in Fig. 4a, does have the required (3 × 2) symmetry and corresponds to the measured cover-

age, the specific atomic ordering within the unit cell is not well established by the experiments. We have proposed a different model, an alternate dimer structure [15], which also satisfies the conditions on symmetry and coverage but has a quite different ordering of the atoms, as shown in Fig. 4b. We have carried out DFT calculations on the two models and find that again both models reduce the surface energy from the (2 × 1)-reconstructed surface, but the alternate dimer structure is significantly more stable than the added dimer structure, by 3.58 eV per ad-dimer! This is a very large energy difference, although since one ad-dimer covers 6 of the (1 × 1) surface cells it amounts to only 0.6 eV per (1 × 1) cell as reported in Table 1.

From our calculation of the added dimer model, the ad-dimer turns out to be symmetric with a bond length of 2.65 Å, suggesting a rather weak interaction. The lengths of the back bonds of the ad-dimer atoms are 2.28 and 2.35 Å, respectively, with the longer one connecting to a second-layer dimer, which has a length of 2.43 Å. The charge density differential indicates the presence of dangling bonds on the ad-dimer atoms.

On the other hand, the ad-dimer in the alternate dimer model is highly asymmetric. In fact, according to our calculation, the tilt between the two atoms in an ad-dimer is very large, 0.52 Å, and the dimer is shifted off-center. The charge density contour plot for this structure in Fig. 5 shows an apparent charge transfer to the higher Si atom, with a dangling bond or lone-pair charge region plainly visible. The dimer bond is also much stronger with a length of 2.28 Å and the length of back bonds that connect the ad-dimers and sublayer dimers is 2.32 Å for the lower atom and 2.40 Å for the upper atom, respectively. The corresponding sublayer dimer length is 2.60 and 2.75 Å, respectively. The unconnected dimer, on the other hand, has a length of 2.29 Å. The stronger surface dimer bonding, as well as some of the dangling bonds on the surface, are also evident in the charge density differentials.

An alternate dimer model for the (5 × 2) structure can similarly be generated with three atom rows in the sublayer separating the dimer rows, but we have not evaluated the energy of this or competing structures.

## 5. Energetics of growth processes

We now briefly address the energetics of some of the growth processes. Creating the $(3 \times 2)$ surface by deposition of disilane, $Si_2H_6$, and release of $H_2$ from the $(2 \times 1)$ surface with no excess of silicon we have (normalized to the $(1 \times 1)$ surface cell):

$$(2 \times 1) + \tfrac{1}{6}Si_2H_6 \rightarrow (3 \times 2) + \tfrac{1}{2}H_2. \qquad (2)$$
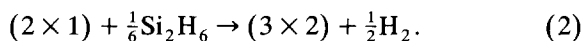
This requires an energy of 0.44 eV in our calculations (2.64 eV per added dimer). This energy may be readily available at typical deposition temperatures – in fact disilane is known to decompose on Si surfaces at those temperatures, and if the reacting molecule is $SiH_2$ rather than $Si_2H_6$ then an energy of 0.50 eV is released in the process of forming the $(3 \times 2)$ structure, according to our calculation.

We also find that deposition of acetylene on the $(3 \times 2)$ surface could, as far as energy is concerned, lead to evaporation of the excess 1/3 coverage Si as proposed by Hara et al. [2]:

$$(3 \times 2) + \tfrac{1}{2}C_2H_2 \rightarrow c(2 \times 2) + \tfrac{1}{6}Si_2H_6, \qquad (3)$$
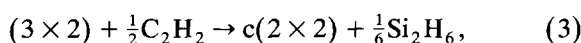
yielding approximately 1.67 eV per $(1 \times 1)$ cell. Even if the final gaseous species is assumed to be $SiH_2$ rather than $Si_2H_6$ (which decomposes into $SiH_2$ and $H_2$ on the surface at these temperatures) the energy gain is still over 0.7 eV. Thereby, a single SiC layer could be formed per growth cycle even though the surface regularly has a 1/3 excess monolayer of silicon.

Deposition of disilane on the $c(2 \times 2)$ C–C-bridged surface is again exothermic

$$c(2 \times 2) + \tfrac{1}{2}Si_2H_6 \rightarrow (2 \times 1) + \tfrac{3}{2}H_2, \qquad (4)$$
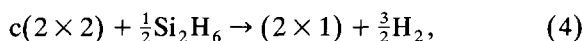
yielding 1.6 eV per $(1 \times 1)$ surface cell. The self-limiting aspect of the growth sequence detailed in these equations can be rationalized from the structures discussed here. The $c(2 \times 2)$ surface has no dangling bonds and is therefore quite inert. The triply bonded carbon pairs do not react with incoming acetylene molecules. On the other hand the Si-terminated $(2 \times 1)$ surface has dangling bonds making it possible that additional Si dimers can cap the bonds as in the alternate dimer $(5 \times 2)$ and $(3 \times 2)$ models. However, a full second layer is not easily formed because of the large lattice mismatch of 25% between SiC and pure Si, and because of the

high deposition temperatures. We have simulated an additional Si monolayer both with DFT calculations and with the Tersoff potential, and find that the extra layer relaxes to a distance of 2.0 Å from the layer below, almost twice the inter-layer distance near the surface for pure silicon. On heating in the Tersoff calculation, some of the atoms leave the top layer to form a third layer on the surface, and the structure appears to be generally unstable, although our simulations did not actually see evaporation from the surface due to the short simulation time.

The alternate dimer model for these surfaces maintains the Si dimerization present in the $(2 \times 1)$ surface so no bond breaking takes place in that layer. Therefore, while the formation of the $(3 \times 2)$ is slightly endothermic (and not at all if disilane is previously decomposed) there is likely not a large energy barrier for this process. When $C_2H_2$ is deposited to form the $c(2 \times 2)$ surface a different dimerization of the Si surface atoms forms. We have observed that there is no barrier to breaking the original Si dimer bonds in the $(2 \times 1)$ surface layer and re-forming them as in the bridged $c(2 \times 2)$ structure.

Recently, we reported a study [15] of the $\beta$-SiC(100) surfaces using the empirical Tersoff potential [16]. There we found that the Tersoff potential correctly predicts the dimer structure of the $(2 \times 1)$ surface. For the $(3 \times 2)$ surface, our new model of alternate dimer rows was found to be energetically more favorable than the added dimer row model of Hara et al. [6]. For the C-terminated $(2 \times 2)$ surface the Tersoff potential favored the staggered dimer model for the $c(2 \times 2)$ surface in contradiction to the DFT results. Since the empirical Tersoff potential is parametrized mainly to reproduce properties of bulk crystals, with no information about surfaces incorporated into the fitting procedure, it is not surprising that it fails to predict the correct surface reconstruction. This illustrates the importance of using ab initio methods in studies of atomic structure of these types of surfaces.

In summary, we have performed ab initio DFT calculations of several atomic models for the $\beta$-SiC(100) surfaces. In particular, for the C-terminated $c(2 \times 2)$ surface, our results favor the model with carbon pairs in the Si bridge sites over the staggered C dimer model. Our calculations also show that for

the excess Si-covered $(3 \times 2)$ surface, the alternate dimer model is much more energetically stable than the added dimer model.

We note that the stability of these surface structures under SiC growth conditions is not solely determined by the energetics. Since the deposition takes place at rather high temperatures it is likely that entropic effects and defects will also influence the surface structure. However, the ab initio calculations of zero-temperature energetics and the associated electronic stucture analysis provide insight into the chemical bonding characteristics which are essential to our understanding of these surfaces.

## Acknowledgements

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