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Ab initio calculations of the 3*C*-SiC(111)/Ti polar interfaces

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Ab initio pseudopotential calculations of 3*C*-SiC(111)/Ti polar interfaces have been performed and compared with *ab initio* calculations of 3*C*-SiC(001)/Ti interfaces [Phys. Rev. B **61**, 2672 (2000)] and the 3*C*-SiC(111)/TiC interface [Phys. Rev. B **55**, 16 472 (1997)] and with experiments on 6*H*-SiC(0001)/Ti interfaces. Two types of interfaces, Si- and C-terminated interfaces, are dealt with in order to examine the dependence on the atom species at the interface. As to stable atomic configurations, the six candidates for each interface are examined. In the most stable configurations, the interfacial Ti atoms are located on top of the center of the triangle of surface atoms of SiC (T_4 site for the Si-terminated interface and H_3 site for the C-terminated interface) rather than on top of surface atoms of SiC (T_1 site). There are serious differences in the bond lengths, bonding nature, and adhesive energies between the Si- and C-terminated (111) interfaces and between the SiC(111)/Ti and SiC(111)/TiC interfaces, respectively. The C-terminated interface has strong interfacial bonds with a large adhesive energy rather than the Si-terminated one, similarly to the (001) interfaces. However, there exist substantial differences between the (111) and (001) interfaces, which can be explained by the interface morphology such as the number of back bonds and the neighboring atoms of interfacial atoms, and the number and direction of surface dangling bonds. A calculated *p*-type Schottky barrier height (SBH) of the C-terminated interface is smaller than that of the Si-terminated one. This SBH relationship is in good agreement with the experimental results of the 6*H*-SiC(0001)/Ti interfaces and consistent with previous *ab initio* results of the 3*C*-SiC(001)/Ti interfaces. The dependence of SBH on the interface atom species can be explained by the following two factors: the relationship of intrinsic band structures between two materials and the interface dipole caused by the interfacial charge distribution. On the other hand, the extended Schottky model has been examined using the theoretical work functions including effects of the surface structure for the SiC(111)/Ti and SiC(001)/Ti interfaces. The obtained relationship of the SBH between the Si- and C-terminated interfaces is contrary to the *ab initio* results and experiments. It is clear that the SBH at the interface is dominated by the interfacial atomic and electronic structures, and is unable to be estimated by the surface properties simply.

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I. INTRODUCTION

Silicon carbide (SiC) is a very attractive material for high-performance (high-temperature, high-speed, high-frequency, and high-power) electronic and optoelectronic devices as well as high-temperature structural ceramics. SiC has a large number of polytypes ($2H, 3C, 4H, 6H, 15R, \ldots$), and each structure has various characters. It is of great importance to fabricate SiC/metal interfaces with desirable properties for various electronic and structural applications of SiC.[1,2] Among them, a SiC/Ti interface is one of the most important systems because Ti or Ti-containing alloys are often used for such applications.[3] The problems of the interfacial orientation and the atom species are important factors to design the structure and properties for the SiC/Ti interfaces. In structural applications, the reactivity between SiC and Ti reveals the anisotropic behavior with respect to the interfacial orientation.[4]

In electronic applications, a Schottky barrier height (SBH) of the SiC/Ti interface[2,5] has been studied extensively as well as the interfacial configurations. The SBH is very important factor to fabricate excellent electronic devices. An extremely low SBH is necessary for an Ohmic contact to achieve a linear current-voltage relationship and a high SBH is required for a rectifying (or Schottky) contact to flow the electric current for only positive or negative voltage bias, such as using a *p-n* junction. The differences in SBH's between the Si- and C-terminated interfaces have been observed in the 6*H*-SiC(0001)/Ti interfaces[6] and the 4*H*-SiC(0001)/Ti interfaces.[7] Recently, *n*-type 6*H*-SiC(0001)/Ti interfaces have been constructed by controlling the density of interfacial defects with special surface treatment.[8] It seems that this kind of experiment reveals the intrinsic nature of the interfacial SBH without the effects of interfacial defects. In this kind of interface, the difference in SBH's between the Si- and C-terminated interfaces has also been observed.[9]

On the other hand, Sugawara and co-workers[10] have found in this kind of interface that Ti on the atomically flat (0001) face of 6*H*-SiC shows a face-centered-cubic (fcc) structure, although the stable structure of bulk Ti is a hexagonal-close-packed (hcp) structure at room temperature. The authors consider that the unusual fcc structure of Ti is due to the high adhesion and high degree of coherence between Ti and SiC. This is expected to be able to control the crystal structure of metal in the future.

From the theoretical point of view, recently, *ab initio* calculations of the 3*C*-SiC(001)/Ti interfaces[11] have been performed using the pseudopotential method based on density functional theory within the local density approximation (DFT-LDA). Both Si- and C-terminated interfaces have been

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examined, and it has been found that both interfaces have quite different features from each other. The Si-terminated interface has weak and metallic Si-Ti bonds, whereas the C-terminated interface has strong and covalent C-Ti bonds such as bulk TiC. The calculated *p*-type SBH of the C-terminated interface is smaller than that of the Si-terminated one. This tendency is consistent with the experiments of 6*H*-SiC(0001)/Ti interfaces[6,9] and 4*H*-SiC(0001)/Ti interfaces.[7] This theoretical result can be explained by the difference in the interface dipoles. Similar theoretical results of the SBH were obtained for the Si- and C-terminated interfaces of the 3*C*-SiC(001)/Al system.[12]

Besides the SiC/Ti system, Rashkeev and co-workers[13] have dealt with the 3*C*-SiC(111)/TiC interface using the full-potential linear-muffin-tin orbital (FP-LMTO) method based on DFT-LDA. In this interface, the arrangement of atom species at the interface layers is similar to the C-terminated SiC(111)/Ti interface, although the C layers are stacked between the Ti layers in the TiC side.

In this paper, we perform *ab initio* calculations of the 3*C*-SiC(111)/Ti polar interface. We use the first-principles pseudopotential method, and obtain the stable atomic configurations, adhesive energies, and SBH's for the Si- and C-terminated interfaces. It is very important to examine such an interface by following reasons.

First, many experiments have been done for the 6*H*-SiC(0001) interfaces.[1,2,5,6,8–10] Especially, some experimental groups make it a challenge to clarify the intrinsic atomic and electronic structures and properties of the 6*H*-SiC(0001)/Ti interface without effects of interfacial defects.[8–10] The theoretical approach is of great importance to be directly compared with such experiments. On the other hand, the 3*C*-SiC(111) interface can be used as a model for the 6*H*-SiC(0001) one because an atomic configuration of the SiC side from the interface to the seventh-layer is similar. According to the preceding calculations of the 3*C*-SiC(001)/metal calculations,[11,12] the properties of coherent interfaces are determined from only a few layers near the interface. Thus, we think that application of the 3*C*-SiC(111) interface as a model of the 6*H*-SiC(0001) one causes no serious problems. The other merit is that the number of atoms in the supercell of *ab initio* calculations can be greatly reduced in dealing with the 3*C*-SiC(111) interface as compared with the 6*H*-SiC(0001) interface. It is of great interest to examine theoretically the difference between the SBH's of the Si- and C-terminated interfaces for the 3*C*-SiC(111)/Ti system, so as to be compared with the experimental results of the 6*H*-SiC(0001)/Ti interfaces.[6,9]

Second, it is of great interest to compare the 3*C*-SiC(111)/Ti interface with the 3*C*-SiC(001)/Ti interface.[11] This comparison should clarify the effect of interface orientation on the interface properties such as the adhesive reaction and SBH. In practical applications, clarification of this effect is one of the most important issues to achieve the hoped for properties. The atomic configurations and properties should depend on the interface orientation through the morphology such as the number of the back bonds and the neighboring atoms at the interface or the number and direction of dangling bonds of each surface.

Third, a comparison between the 3*C*-SiC(111)/Ti interface and the 3*C*-SiC(111)/TiC interface[13] with respect to the stable atomic configuration and the SBH is also of great interest. Particularly, many experiments are uncertain whether TiC layers are formed at the SiC/Ti interface or not. Thus, this comparison should clarify the features of interfaces with and without TiC layers, theoretically.

In this paper, we also perform a detailed discussion of the mechanism of the SBH using the results of the SiC(111)/Ti and SiC(001)/Ti interfaces. Here, we briefly explain previous traditional models of the mechanism of the SBH of semiconductor/metal or ceramics/metal interfaces. First, the Schottky model[14] evaluates the SBH by the difference between the work function of metal and the electron affinity of a semiconductor or ceramics. In this model, the SBH should be changed in proportion to the change of the work function of metal for the same semiconductor. However, the SBH's of several semiconductors such as Si and GaAs are experimentally observed to be only a little changed.[15] This phenomenon is explained by the Fermi level pinning by some specific states in the band gap of semiconductor at the interface, for example the states associated with defects.[16,17] On the other hand, the metal-induced gap state (MIGS) and charge neutrality level (CNL) model[18] proposes that the SBH is determined by occupying electrons up to the CNL within the MIGS (Ref. 19) at the interface, which are formed in the band gap of semiconductor. The CNL is considered to be intrinsic to respective semiconductors.

In this paper, we concentrate on the intrinsic nature of the SBH without the effects of interfacial defects, because our *ab initio* calculations can deal with only coherent interfaces without any defects. On the other hand, such an intrinsic SBH is tried to be examined experimentally.[8,9] From this point of view, the Schottky model and MIGS-CNL model are influential. However, these two models deny that the SBH depends on the practical interface structure. Hence, these models cannot explain well the experimental and theoretical results of the SBH's with the interface-structure dependence for $\mathrm{NiSi_2}$/Si interfaces[20–22] and for SiC/metal interfaces.[11,12] Our preceding *ab initio* calculations[11] have indicated that an intrinsic SBH of the interface without any defects is determined by ‘‘two factors’’ in a similar way as the band discontinuity of the semiconductor heterojunction: (i) the relationship of intrinsic band structures between two materials and (ii) the interface dipole derived from the charge transfer or the charge distribution itself at the interface. The latter depends on the interface structure, whereas the former does not. If we consider a surface as an interface between vacuum and material, the ‘‘two factors,’’ the band-structure term and the dipole term, should correspond to the two dominant factors of the work function of the surface. It is of great interest to compare the calculated SBH's of the present Si- and C-terminated 3*C*-SiC(111)/Ti interfaces with those of the (001) interfaces and with the two-factor model, the Schottky model, and the MIGS-CNL model.

On the other hand, recent experiments of the 6*H*-SiC(0001)/metal interfaces with reduced defect density seem to indicate that the SBH behaves as a Schottky limit for various metals.[8] Thus, we additionally examine the extended

Schottky model. The work function (electron affinity) in the original Schottky model is defined as an intrinsic constant for each material. However, the work function (electron affinity) itself depends on the surface structure as revealed in many surface calculations. Then, we examine the SBH's estimated from *ab initio* calculations of the work function of each surface slab for the SiC(111)/Ti and SiC(001)/Ti interfaces. As shown below, the result indicates that the interface property cannot be predicted correctly by the sum of properties of two surfaces or two materials.

II. THEORETICAL METHOD

First of all, it is necessary to overcome several tough problems associated with the (111) polar interfaces as compared with the (001) interfaces.[11] In the periodic cell, the atom species of both surfaces on the $3C$-SiC(111) slab cannot be the same, because the slab, the basic structure of which is zinc blende, does not have a mirror plane and inversion center. This is quite different from the case of the SiC(001) slab. If we use the original (111) slab, charge transfer will occur between two surfaces or between two interfaces, and an electric-field problem will rise, which should prevent realistic calculations. Even if the charge transfer is suppressed, it is not so easy to analyze the energy of the respective interface regions in the supercell containing two different interfaces. In order to settle this problem, we construct a slab with two identical (111) surfaces by introducing a stacking fault at the center of the SiC slab. The slab has mirror-plane symmetry with respect to the center of the stacking fault. At the stacking fault, Si-Si or C-C wrong bonds are introduced. However, these wrong bonds do not create deep levels in the band gap or any extra carriers because SiC is a homovalent compound, as observed in *ab initio* calculations of the SiC grain boundaries.[23] As will be shown, the existence of the stacking fault does not seem to have serious effects on the interfaces. The same kind of stacking fault has been introduced in the calculation of the $3C$-SiC(111)/TiC interface,[13] as inversion domain boundaries.

The supercell of the interface consists of a slab of 16 SiC(111) atomic layers including one stacking fault and two sets of 4 Ti(111) layers stacked on both SiC surfaces. In this paper, we deal with a coherent (1×1) interface, where Ti layers are slightly expanded parallel to the interface. The Ti layers have fcc structure similarly to our preceding study of the SiC(001)/Ti interface,[11] although the hcp structure is stable as the bulk structure at room temperature. As mentioned in Sec. I, the recent high-resolution transmission electron microscopy (HRTEM) observation[10] found that fcc-Ti is generated on the atomically flat (0001) face of $6H$-SiC at room temperature, where the orientation relationship between the fcc-Ti and the $6H$-SiC substrate is $(111)_{\text{fcc-Ti}}//(0001)_{\text{6H−SiC}}$ and $[\bar{1}10]_{\text{fcc-Ti}}//[11\bar{2}0]_{\text{6H-SiC}}$. From the analysis using coincidence of reciprocal lattice points,[10] the orientation relationship has high coherency across the interface and a lattice mismatch between fcc-Ti and $6H$-SiC is very small ($<1\%$) in comparison with the hcp-Ti/6H-SiC system ($\sim 4.3\%$). Our preliminary first-principles calculations, the pseudopotential method, and the full-potential linearized augmented plane-wave method, for bulk Ti, indicate that the difference of total energy between fcc-Ti and hcp-Ti is very small (<10 meV/atom).[24]

In the supercell, a vacuum region more than 15 a.u. separates two free metal surfaces, which ensures stable interlayer distances without any constraint. About the determination of a stable position of a Ti layers parallel to the interface and the stable stacking sequence of the Ti layers, we examine six candidates of special translations corresponding to energy extrema as shown in next section. All the configurations have special symmetry of the point group D_{3h}.

Interface structures are obtained by *ab initio* pseudopotential calculations based on DFT-LDA (Ref. 25) for the above supercell. To obtain the electronic ground state, a conjugate-gradient technique[26] and an effective charge-mixing scheme[27] for controlling the charge-sloshing instability[28] are used. Stable atomic configurations are obtained through the relaxation according to Hellmann-Feynman forces. Present pseudopotentials are softened by a Troullier-Martins-type optimization.[29] The Kleinman-Bylander separable form[30] is used with the local p component for Si and for C and with the local s component for Ti. A plane-wave cutoff energy of 50 Ry is used. In self-consistent calculations, 16 $\mathbf{k}$ points in the irreducible 1/24 Brillouine zone are used.

In the present system, there is other difficulty about the stability of the self-consistent iterations. The present supercell is extremely slender, as compared with the supercell for the SiC(001)/Ti interface. The ratio of cell size normal to the interface, c, to that parallel to the interface, a, i.e., c/a, is about 15. In such a type of supercell, the convergence of the self-consistent loop of the charge density is not so easy even if we use the efficient charge-mixing scheme.[27] In order to execute huge computations of the self-consistent loop of large supercells, we used a parallel-type supercomputer by developing a program code using the message-passing interface (MPI).

III. ATOMIC MODEL

As to the rigid-body translations parallel to the interface between the Ti layers and the SiC surface, a high-symmetry configuration should correspond to the total energy extrema. Thus, we examine three groups of atomic configurations with threefold symmetry for both the Si- and C-terminated interfaces as shown in Fig. 1: (i) Ti on top of the surface atoms of SiC (case 1 and case 2), denoted by T_1, (ii) Ti above the hollow site of SiC (case 3 and case 4), denoted by H_3, and (iii) Ti above the second-layer atoms of SiC (case 5 and case 6), denoted by T_4. The difference in each pair is the stacking position of the second-layer Ti because a stacking of fcc type has two candidates about the second-layer atoms as $ABCA\ldots$ and $ACBA\ldots$. In the T_1 group, an interfacial Ti atom interacts directly with a dangling bond of each Si or C atom, and hence each Ti atom has only one neighboring Si or C atom. In this case, it seems that the bonding nature between interfacial atoms is dimer like. On the other hand, in the two other groups H_3 and T_4, the interfacial Ti atoms are located on top of the center of the triangle of surface atoms

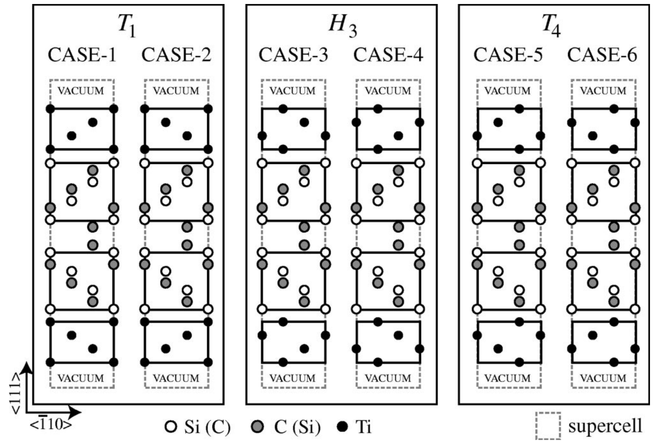

FIG. 1. Atomic models of the $3C$-SiC(111)/Ti interface (cases 1–6).

TABLE I. Distance between atoms near the Si- and C-terminated (111) and (001) interfaces (Ref. 11). "Si-C(back)" and "Ti(int)-Ti" indicate a bond between interfacial Si (C) and back C (Si) atom and an interfacial Ti atom, respectively. A unit of data is a.u.

	Interface	Si-C(back)	Ti(int)-Ti
(111)			
Si-terminated	4.97	3.57	5.66
C-terminated	4.37	3.59	5.84
(001)[a]			
Si-terminated	4.79	3.52	4.87
C-terminated	3.83	3.54	5.32

[a] Reference 11.

of SiC, and hence each Ti atom interacts mainly with three neighboring Si or C atoms. Also the interfacial Si or C atoms have three neighboring Ti atoms. The difference between H_3 and T_4 is the back side of the SiC. In T_4, there exists the second-layer atom (Si or C) near the interfacial Ti atom, while no existence in H_3. Thus it may be possible that the interfacial Ti atom interacts with the interfacial Si or C atoms and the second-layer C or Si atom in T_4.

IV. RESULTS AND DISCUSSION

A. Atomic configurations

The most stable configurations for the Si- and C-terminated interfaces are determined by the relaxation of all six candidates (case 1 to case 6) of atomic configurations. First of all, the total energy difference within each group is very small (<0.01 Ry per supercell). Thus, the difference in stacking sequences after the second Ti layer does not create a large energy difference. This feature may be related to the growth of Ti layers with fcc structure instead of hcp structure observed experimentally.[10] In both the Si- and C-terminated interfaces, the total energies of two T_1 configurations (case 1 and case 2) are considerably higher than those of the other groups (>0.1 Ry per supercell), which means that these configurations are unstable or metastable rather than the others.

In the Si-terminated interface, the configurations of T_4 are more stable than those of H_3. And case 5 and case 4 are more stable in T_4 and H_3, respectively. Therefore, case 5 is the most stable. As listed in Table I, the Si-Ti distance, 4.97 a.u., in case 5 is comparable with a range of the Si-Ti distance in Ti silicide, 4.91–5.29 a.u.[31] It should be noted that the distance of the second-layer C and the interfacial Ti, 4.88 a.u., is rather small, although this is larger than the C-Ti bond length in bulk TiC, 4.08 a.u. There exists a strong adhesive interaction between C and Ti atoms in the SiC(001)/Ti system.[11] Thus, it has the possibility that the interaction between the interfacial Ti and the second-layer C exists in addition to the interaction between Ti and Si in case 5. In case 4, on the other hand, the Si-Ti distance, 5.01 a.u., is close to that of case 5, while interfacial Ti is far from the second-layer C. Thus, case 5 should be more stable than case 4 for the Si-terminated interface.

In the C-terminated interface, on the other hand, H_3 (case 4) is more stable than T_4 (case 5) contrary to the Si-terminated one, where case 5 is more stable in T_4, and case 4 is more stable in H_3. The C-Ti distance is 4.37 a.u. in case 4 and 4.50 a.u. in case 5, respectively. These values are close to the bulk TiC (4.08 a.u.), but slightly larger. In case 5, the distance of the second-layer Si and interfacial Ti is 4.25 a.u. This is too small as compared with the range of the Si-Ti distance in Ti silicide, which is caused by the small interfacial C-Ti distance. The interaction between Ti and the second-layer Si should behave as repulsive, which results in the C-Ti distance in case 5 larger than that in case 4. Thus, case 4 with no repulsive interaction between Ti and the second-layer Si is more stable. In this way, case 5 and case 4 are the most stable for the Si- and C-terminated interfaces, respectively. From here on, we discuss the atomic and electronic structures of these configurations.

As listed in Table I, the Si-Ti distance of the Si-terminated interface is larger than the C-Ti distance of the C-terminated one. The Si-Ti and C-Ti distances of the Si- and C-terminated interfaces are larger than those of the (001) interfaces, respectively, which is concerned with the number of neighboring atoms at the interface as discussed below. The back Si-C bond lengths of both the Si- and C-terminated interfaces are similar values to the Si-C bond length in bulk $3C$-SiC, 3.57 a.u., such as the (001) interfaces. In both the Si- and C-terminated interfaces, the interlayer distance at the interface is quite smaller than that between the interfacial Ti and back Ti layers, as listed in Table II. The interlayer distance between the interfacial Ti and second Ti layers of the Si-terminated interface, 4.56 a.u., is smaller than that of the C-terminated one, 4.77 a.u. This is because the interfacial Ti layer of the C-terminated interface is attracted to the SiC surface greater than that of the Si-terminated interface as seen below.

Figure 2 shows the stable atomic configurations and the valence-charge distributions on the $[\bar{1}10]$ cross sections for the Si- and C-terminated interfaces. In the Si-terminated interface of Fig. 2(a), the charge distribution around the inter-

TABLE II. Interlayer distance of the Si- and C-terminated (111) interfaces. "int." and "S.F." mean the interfacial atom and the stacking-fault atom, respectively. A unit of data is a.u.

	Si-terminated interface	C-terminated interface
Ti(third to fourth)	4.16	4.22
Ti(second to third)	4.89	4.76
Ti(int. to second)	4.56	4.77
Interface	3.71	2.79
SiC(int. to second)	1.20	1.25
SiC(second to third)	3.58	3.53
SiC(third to fourth)	1.19	1.20
SiC(fourth to fifth)	3.58	3.56
SiC(fifth to sixth)	1.18	1.19
SiC(sixth to seventh)	3.67	3.54
SiC(seventh to S.F.)	1.25	1.18
Between S.F.	3.08	4.42

facial Ti atom has no drastic changes as compared with the other Ti atoms, although there exist some changes at the interfacial Ti atom and a slight increase of the charge density at the Si-Ti bond. It can be said that the Si-Ti bond has rather metallic character with rather broadly distributed charge density. This feature is similar to the Si-Ti bond of the Si-terminated interface of the SiC(001)/Ti system,[11] although the atomic structure is different.

In the C-terminated interface of Fig. 2(b), the charge distribution around the interfacial Ti atom has substantially different features from the other Ti atoms. The C-Ti bond length is very small. It is clear that the Ti (111) and C (111) layers are closely stacked at the interface with some similarity with the (111) stacking layers in bulk TiC. There exist increases in the charge distribution between the Ti and C atoms. There seems to exist both covalent and ionic interactions between Ti and C atoms, similarly to the SiC(001)/Ti interface.[11] This point is not so clear from the present figure, as compared with the case of the SiC(001)/Ti interface where *p-d* hybridization like bulk TiC can be seen. However, this point will be shown in the local density of states (LDOS) analysis.

The difference of the charge distribution for respective Si-Ti and C-Ti bonds between the (111) and (001) interfaces can be explained by the numbers of neighboring atoms at the interface and the numbers of back bonds of each interface atom. This problem will be discussed later.

The bond lengths of the C-C and Si-Si bonds at the stacking faults of the Si- and C-terminated interfaces are 3.08 a.u. and 4.42 a.u., respectively, as results of free relaxation. These values are near the bond length in diamond, 2.92 a.u., and in bulk Si, 4.44 a.u. Thus, it does not seem that these wrong bonds generate structural or electronic frustration affecting the interface regions in the supercell. In the SiC(001)/Ti interface,[11] the 9 SiC(001) atomic layers of the supercell are expanded along the $\langle 001\rangle$ direction; especially the total expansion of the C-terminated one is rather large, 3.7%. However, in the present interfaces the total expansion of the 14 SiC(111) atomic layers of the surpercell except for the stacking fault is less than 1% of both the Si- and C-terminated interfaces. This small distortion means that the influence of interface formation and the stacking fault on the SiC bulk region is rather small.

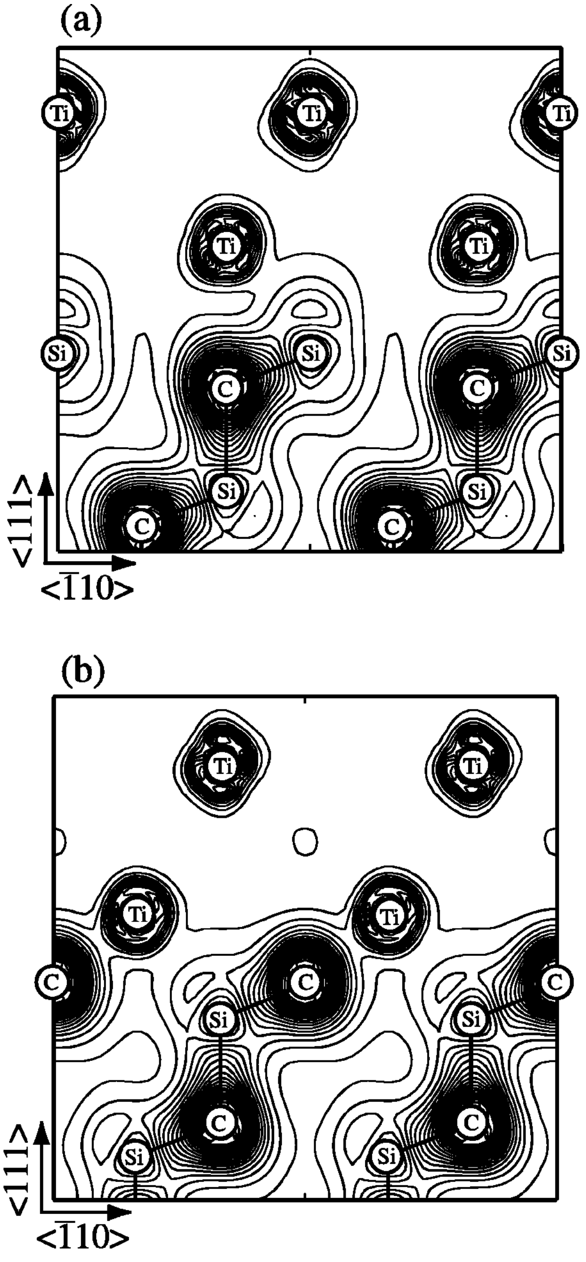

FIG. 2. Stable atomic configuration and charge distribution of (a) the Si-terminated and (b) the C-terminated 3*C*-SiC(111)/Ti interfaces. $[\bar{1}10]$ cross sections are shown. All atoms are located on the same $(\bar{1}10)$ plane. Contours of the charge density is plotted from 0.001 a.u.$^{-3}$ to 0.281 a.u.$^{-3}$ for the Si-terminated one and from 0.001 a.u.$^{-3}$ to 0.288 a.u.$^{-3}$ for the C-terminated one in spacing of 0.015 a.u.$^{-3}$

In comparison with the *ab initio* calculation of the 6*H*-SiC(0001) surface,[32] the interlayer distances of the back Si-C layers of the Si- and C-terminated interfaces, 1.20 a.u. and 1.24 a.u., as listed Table II, are similar to the interlayer distance of the (1×1) ideal unit cell, 1.19 a.u., and are much larger than those of the relaxed (1×1) Si- and C-terminated surfaces, 0.91 a.u. and 0.71 a.u., because of the formation of interfacial bonds. The interlayer distances of the second to third SiC layers of the Si- and C-terminated interfaces, 3.58 a.u. and 3.53 a.u., are slightly smaller than those of the relaxed Si- and C-surfaces, 3.70 a.u. and 3.72 a.u.

About the comparison with the SiC(111)/TiC interface,[13] three kinds of configurations of the interface corresponding to the H_3 (case 3 and case 4) and T_4 (case 6) groups of the C-terminated SiC(111)/Ti interface in the present models were examined in Ref. 13, although the C layers are stacked between the Ti layers in the TiC side. The reason why only the C-terminated interface is dealed with in Ref. 13 is that the formation of the Si-Ti bond at the SiC(111)/TiC interface seems to be unfavorable because both the Ti and Si atoms play the role of cation in TiC and SiC. In Ref. 13, T_4 (case 6) is found to be metastable with a significantly higher energy than H_3, although the difference of total energies within H_3 group (case 3 and case 4) is rather small (8 meV/atom). It is of great interest that the relative stability among these three models for the SiC/TiC system is similar to our results for the SiC/Ti interface. The interfacial C-Ti distance (4.37 a.u.) in the most stable case 4 of the SiC(111)/Ti interface is larger than the interfacial C-Ti bond length (4.05 a.u.) in the most stable structure of the SiC(111)/TiC interface.[13] The latter is very close to that of bulk TiC (4.08 a.u.). In the SiC(111)/TiC interface, the interfacial Ti atom is a part of TiC, where the partial charge transfer from Ti to C already exists in the TiC side. In the SiC(111)/Ti interface, on the other hand, the back side of the interfacial Ti atom is metallic Ti. This should be the reason why the bond length at the SiC/Ti interface is larger.

B. Electronic structure

Figure 3 shows an averaged charge density on each (111) plane plotted along the ⟨111⟩ axis. In the Si-terminated interface, the slope is changed in the SiC side near the interface. However, it seems that the averaged charge density at the interface has a feature like simple superposition of the charges of Ti and Si layers. This is consistent with the rather weak interactions observed in Fig. 2(a). In comparison with the (001) interface,[11] there exists no fine structure in the averaged charge at the interface, which may be associated with the small interlayer distance at the interface.

In the C-terminated interface, the charge of the interfacial Ti layer is merged into the shoulder of the charge of the C layer, because of a very small interlayer distance. And there exists the charge-depletion region between the interfacial Ti and back Ti layers. In the (001) interface, the charge transfer from Ti to C was observed obviously. In the (111) interface, on the other hand, the charge transfer from Ti to C is not so clear. This is because the charge density of the interfacial Ti layer overlaps that of the C layer by the small interlayer distance as mentioned above. However, the charge of the C layer is slightly larger than that of the SiC bulk region. This feature shows the possibility of charge transfer from Ti to C.

Figure 4 shows the LDOS for each (111) interface. The LDOS is calculated for each region between successive (111) layers of the supercell. Eigenstates for 16 **k** points in the irreducible part are broadened with a Gaussian half width (0.16 eV) similarly to the (001) interface.[11] It should be noted that a too large broadening width may affect the analysis of MIGS's because of the large shoulders of the band edges.

In the Si-terminated interface, the LDOS at the interface region seems to have a feature like the superposition of the DOS of SiC and Ti, similarly to the Si-terminated (001) interface.[11] This is consistent with the metallic character of the Si-Ti bond observed in the charge-density distribution in Fig. 2(a). However, there exists a sharp peak near the top of the SiC valence band and there exists a decreased region near

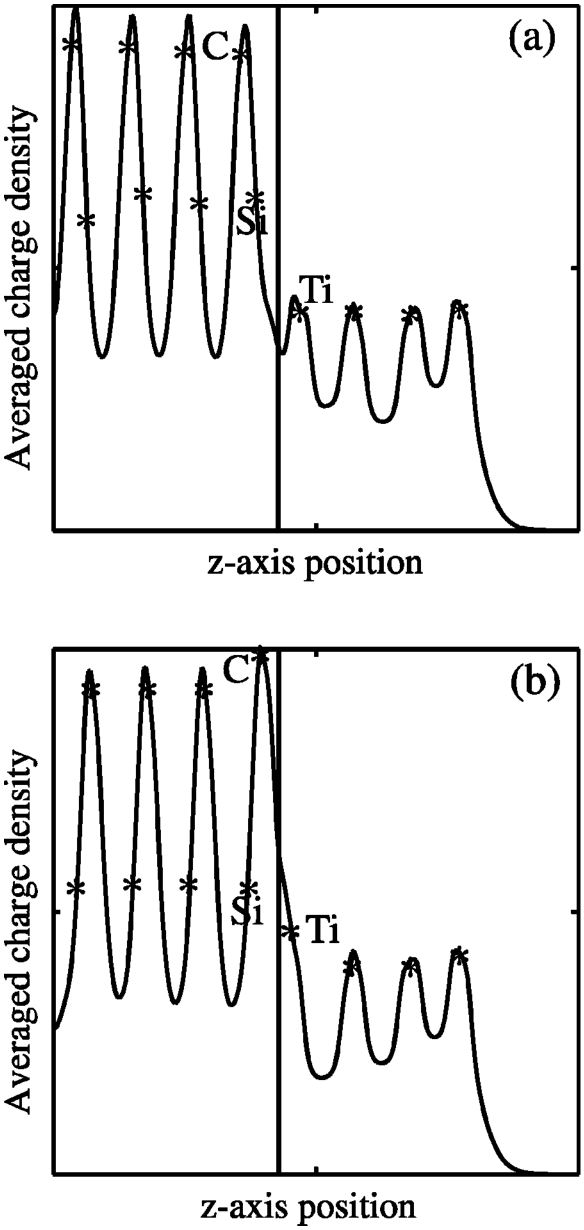

FIG. 3. Averaged charge density profile along the ⟨111⟩ axis of (a) the Si-terminated and (b) the C-terminated 3*C*s-SiC(111)/Ti interfaces. The half of the supercell containing four sets of SiC layers and four Ti layers with the vacuum region is shown. Asterisks indicate the positions of atomic layers. A vertical line indicates the interface.

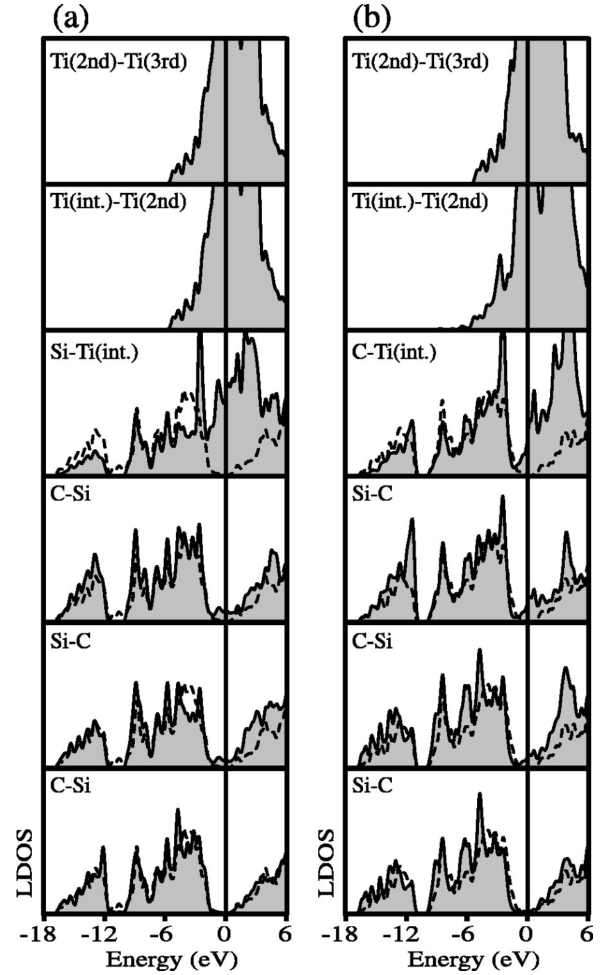

FIG. 4. Local density of states (LDOS) for (a) Si- and (b) C-terminated 3*C*-SiC(111)/Ti interfaces. The LDOS is given for each region between successive (111) atomic layers. Dashed lines indicate the LDOS of the bulk SiC region in the supercell. A vertical line indicates the Fermi level.

TABLE III. Calculated adhesive energy and *p*-type SBH for the Si- and C-terminated (111) and (001) interfaces (Ref. 11) and experimental *p*-type SBH ($\mathrm{SBH_{expt}}$) for the Si- and C-terminated 6*H*-SiC(0001)/Ti interfaces (Refs. 6 and 9). Adhesive energy is the energy gain by the interface formation from relaxed surfaces.

	Adhesive energy [eV/(1×1) cell]	Adhesive energy [J/m^2]	SBH [eV]	$\mathrm{SBH_{expt}}$ [eV]	$\mathrm{SBH_{expt}}$ [eV]
(111)					
Si-terminated	3.21	6.25	1.02	2.16[a]	2.549[b]
C-terminated	3.88	7.56	0.67	1.79[a]	1.903[b]
(001)[c]					
Si-terminated	1.48	2.52	0.50		
C-terminated	5.11	8.74	0.22		

[a] Reference 6.
[b] Reference 9.
[c] Reference 11.

the Fermi level, differently from the Si-terminated (001) interface. This means the partial covalent nature of the Si-Ti bond. The LDOS recovers the bulk features at the regions of back C-Si and Ti-Ti interlayer. In the C-terminated interface, the LDOS at the interface region has a deep valley near the Fermi level. A similar valley was also observed in the LDOS of the (001) interface. This kind of valley represents both covalent and ionic interactions of the C-Ti bond.

One of the important factors in the LDOS analysis is the MIGS. The MIGS-CNL model[18] insists that the existence of MIGS's affects the SBH seriously. As seen in Fig. 4, MIGS's seem to exist in the band gap up to the second Si-C layers near the interface as tiny peaks in both the interfaces. Similar peaks were observed in the (001) interfaces.[11] We think that these MIGS peaks are tails of metallic Ti states or tails of hybridization between dangling bonds and Ti orbitals. In both the Si- and C-terminated (111) interfaces, the MIGS peaks are smaller than those of the (001) interfaces, and disappear rather quickly at the third layer as compared with those of the (001) interfaces. These points may be concerned with only one dangling bond per (111) surface atom as compared with two dangling bonds per (001) surface atom.

In comparison with the LDOS of the SiC(111)/TiC interface,[13] the MIGS's of the SiC(111)/TiC interface are similar to those of the SiC(111)/Ti interface. And the MIGS's of the SiC(111)/TiC interface rapidly decrease inside the SiC region similarly to the SiC(111)/Ti interface.

C. Adhesive energy

An adhesive energy is energy gain by the formation of an interface from two free surfaces and is obtained from the difference in total energies between the relaxed interface and relaxed (1×1) Si- or C-terminated SiC and Ti surfaces, using supercells with the same size. Results are listed in Table III with those of the (001) interfaces.[11] In the (111) interfaces, the value of the C-terminated interface is larger than that of the Si-terminated one, similarly to the (001) interfaces. This means that the interfacial bond at the C-terminated interface is stronger than that at the Si-terminated one. As to the comparison with the (001) interfaces, the adhesive energy of the Si-terminated (111) interface is quite larger than that of the Si-terminated (001) one, while the adhesive energy of the C-terminated (111) interface is smaller than that of the C-terminated (001) one. Thus, for the Si-terminated interfaces, the interfacial adhesion of the (111) interface is stronger than that of the (001) one, contrary to the C-terminated interfaces.

Here we summarize the bonding nature of the present (111) interfaces in order to discuss the adhesion results. The Si-Ti bond of the Si-terminated interface is metallic and partially covalent as shown in the charge distribution of Fig. 2(a) and the shape of the LDOS of Fig. 4(a). This feature is basically similar to the (001) interface.[11] It should be noted that the Si-Ti bond length and the number of neighboring atoms are similar to the Ti silicide.[31] On the other hand, the C-Ti bond of the C-terminated interface is covalent and ionic as shown in the charge distribution of Fig. 2(b) and the shape of the LDOS of Fig. 4(b). This feature is similar to bulk TiC.

And the number of neighboring atoms and C-Ti bond lengths is also similar to bulk TiC. These are basically similar to the (001) interface.

However, the Si- and C-terminated (111) interfaces have substantially different features from those of the (001) interfaces. For the C-terminated (111) interface, the C-Ti bond length is larger than that of the (001) interface, and the charge transfer and *p*-*d* hybridization are not so noticeable as compared with the (001) interface. In both the (111) and (001) interfaces, the adhesive energies of the C-terminated interfaces are larger than those of the Si-terminated interfaces, which can be understood by the difference in the bonding nature. However, the adhesion of the Si-terminated (111) interface is stronger than that of the Si-terminated (001) one, while the adhesion of the C-terminated (111) interface is weaker than that of the C-terminated (001) one, as mentioned above.

The difference between the (111) and (001) interfaces can be explained as follows. As for the C-terminated interfaces, both the interfaces tend to form local configurations like TiC. From the number of the C-Si back bonds and the C-Ti interfacial bonds for the interfacial C atom, it is clear that the interfacial C atom of the (111) interface and that of the (001) interface are located in the environment more close to SiC and close to TiC, respectively. In the (001) interface, a zigzag-chain structure of C-Ti bonds is formed parallel to the interface, which is similar to the local configuration of bulk TiC. The C atom on the (001) surface has two back bonds with back Si atoms and has two dangling bonds, which form strong covalent and ionic bonds with two neighboring Ti atoms at the interface. In the (111) interface, on the other hand, the stacking of the interfacial layers is similar to that of the TiC (111) layers. However, the C atom on the (111) surface has three back bonds with back Si atoms and has only one dangling bond. The dangling bond connects with the three interfacial Ti atoms at the interface.

In this way, the interfacial C-Ti layers of the (001) interface tend to have atomic and electronic structures closer to bulk TiC rather than that of the (111) one. This is the first reason why the (001) interface has a larger adhesive energy than the (111) interface. This point is consisted with the calculated results of bond lengths, charge distribution, and LDOS.

The second reason why the adhesive energy of the C-terminated (001) interface is larger than that of the C-terminated (111) interface is that both surface energies of the SiC and Ti (001) slabs are larger than those of the (111) slabs. For instance, the number of dangling bonds per surface atom of the SiC (111) and (001) surfaces are 1 and 2, respectively, the coordination numbers of the Ti (111) and (001) surfaces are 9 and 8, respectively, and 12 in the bulk Ti.

As for the Si-terminated interfaces, the (001) interface has the zigzag-chain structure of the Si-Ti bonds similarly to the C-terminated interface. And the (111) interface also has a stacking of interfacial layers similarly to the C-terminated interface. It can be said that the local configuration at the (111) interface has features closer to Ti silicide than that at the (001) one. Such a configuration that the interfacial Si atom has many interacting Ti atoms seems to be favorable for the interfacial metallic and partially covalent bonding like Ti silicide. This should be the reason why the (111) interface has a larger adhesive energy than the (001) interface for the Si-terminated interface. In addition, the interaction between the interfacial Ti atoms and the second-layer C atom affects the adhesion of the (111) interface.

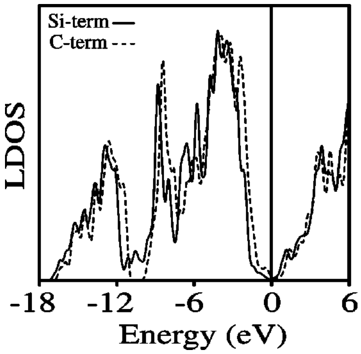

FIG. 5. Local density of states (LDOS) of the bulk region of the Si- and C-terminated 3*C*-SiC(111)/Ti interfaces. A vertical line indicates the Fermi level.

D. Schottky barrier height

A *p*-type SBH can be obtained by supercell calculation as the difference between the Fermi level of the supercell and the valence-band top (VBT) of the bulk SiC region.[11,12] It should be noted that no band bending occurs in the present supercell calculations because of no dopants and zero temperature. Thus, the Fermi level only means the highest occupied level of the metal region, which should be located somewhere in the band gap of the bulk SiC region. There exists a step for the highest occupied states from the VBT of the bulk SiC region to the Fermi level of the metal region. This step corresponds to the *p*-type SBH. The VBT of the bulk SiC region is determined by analysis of the LDOS. Of course, as shown in Fig. 5, the shape of the LDOS of the bulk SiC region has some disorder especially near the VBT by the influence of the interface. Thus, the VBT is determined by comparing the LDOS with the DOS of the bulk crystal, where the valence-band bottom (VBB) is first determined by fitting the main peaks of the LDOS to those of the bulk DOS.

Calculated SBH's are listed in Table III with those of the (001) interface.[11] The values of the *p*-type SBH's for the Si- and C-terminated interfaces are 1.02 eV and 0.67 eV, respectively, and the difference is 0.35 eV. In Fig. 5, the shift of the valence band of the bulk SiC region of the C-terminated interface against that of the Si-terminated one is clearly seen, which corresponds to the difference in the SBH. The tendency of the value of the C-terminated interface to be lower is similar to the (001) interfaces.

LDOS's near the interfacial region have MIGS's as shown in Fig. 4. In the present *ab initio* calculations as well as those of the SiC(001)/Ti (Ref. 11) and SiC(001)/Al interfaces,[12] it does not seem that the MIGS's have dominant effects to determine the SBH of respective interfaces.

In comparison with experiments, the *n*-type SBH of the Si-terminated 6*H*-SiC(0001)/Ti interface is 0.79–0.88 eV for as-deposited contacts.[5] This means a *p*-type value of 2.1–2.2 eV using the experimental band-gap value (3.0 eV). Our calculated SBH of the Si-terminated interface is much smaller than this. In DFT-LDA calculations, there is the problem of possible discontinuity in the exchange-correlation potential across the interface between different materials.[20] In 3*C*-SiC, such a problem has been discussed and the value (−0.66 eV) for the correction to the VBT is obtained.[13,33] Thus, it may be difficult to estimate the SBH quantitatively in the present calculations. However, the difference in SBH's for the Si- and C-terminated interfaces and the qualitative properties should be reliable.

Waldrop and Grant[6] have reported the SBH of *n*-type 6*H*-SiC(0001)/metal (Pd, Au, Ag, Tb, Er, Mn, Al, Ti, Ni, and Mg) and *p*-type 6*H*-SiC(0001)/metal (Pd, Ni, Au, Ag, Mg, Ti, and Al) systems with respect to both Si- and C-terminated interfaces. Generally, the *n*-type SBH of the C-terminated interface is larger than that of the Si-terminated one, while the opposite relationship exists for the *p*-type SBH, except for Au, Ag, and Mg. The dependence on the termination atom species is obvious for 6*H*-SiC(0001)/metal systems. The SBH's of the Si- and C-terminated 6*H*-SiC(0001)/Ti interfaces[6] are 0.73–0.75 eV and 1.0–1.09 eV for the *n*-type SBH, respectively, and 2.16 eV and 1.79 eV for the *p*-type SBH, respectively. The differences between the Si- and C-terminated interfaces are 0.27–0.34 eV for the *n*-type SBH and 0.37 eV for the *p*-type SBH. These difference values are in good agreement with our result, 0.35 eV. In the 4*H*-SiC(0001)/Ti interfaces,[7] the *n*-type SBH's of the Si- and C-terminated interfaces are 0.95–1.09 eV and 1.16–1.25 eV, respectively. The relationship of SBH's between the interface species is similar to our result.

Of course, it is necessary to consider the effects of interfacial defects or the formation of reaction layers in a comparison between the experimental SBH's and the present calculated ones. Recently, the 6*H*-SiC(0001)/metal interfaces with greatly reduced density of interfacial defects have been fabricated through special surface treatment, and the SBH's of such atomically flat interfaces have been examined.[8,9] For the *n*-type 6*H*-SiC(0001)/Ti interface in such experiments, the values of the SBH's of the Si- and C-terminated interfaces are 0.451 eV and 1.097 eV for as-deposited contacts, respectively,[9] which correspond to 2.549 eV and 1.903 eV for the *p*-type SBH using the experimental gap value. The difference of the SBH's between the Si- and C-terminated interfaces is 0.646 eV.

The present calculated results of the SBH depending on the interface structure can be explained by the following two factors in a way similar to the SiC(001)/metal interfaces[11,12]: first the relationship of the intrinsic band structures of the two materials, independent of the interface structure, and second the interface dipole caused by charge transfer or the charge distribution itself at the interface, depending on the interface structure. We think that these two factors should generally determine the intrinsic SBH's of the two materials without any effects of defects. This idea is consistent with the theoretical and experimental results of the $NiSi_2/Si$ interface[20–22] as mentioned in Sec. I. In the case of the C-terminated SiC(001)/Ti interface,[11] the interface dipole lowering the *p*-type SBH is clearly caused by the charge transfer from the interfacial Ti layer to the interfacial C layer. In the present C-terminated (111) interface, such charge transfer is not so clear in Fig. 4. However, the charge density at the interfacial C layer is increased because of the C-Ti bond formation. This may be associated with the formation of an interface dipole lowering the electrostatic potential of the Ti side, resulting in the present smaller value of the *p*-type SBH.

In the SiC(111)/TiC interface,[13] the *p*-type SBH is calculated by two types of methods. In one method, the VBT of the bulk SiC region and the Fermi level of the TiC region are determined from the lineup of the core levels of each atomic layer in the supercell. The *p*-type SBH is obtained as the difference between the VBT and the Fermi level similarly to our method. The obtained value is 1.1 eV without the LDA correction. In the other method, analyzing the LDOS similarly to our method, the SBH value is 0.9 ± 0.1 eV. These SBH's are larger than that of the present C-terminated interface. This point is reasonable if we consider the larger charge transfer from Ti layers than that from TiC layers.

Next, we discuss the effects of dopants in semiconductors on the SBH. The *n*- or *p*-type dopants exist in the usual SiC samples in SBH experiments. If some dopants exist in the semiconductor in a real system, the charge of dopants near the interface should go to the interface, which generates a macroscopic dipole associated with the band bending and depletion regions. However, for the usual dopant concentration, the amount of the accumulated charge and the electrostatic potential in the depletion layer should be extremely small for the area of the interface in the atomic scale. Thus, the shape of the LDOS of the interface and the occupation should be little changed for the formation of such a macroscopic dipole. Therefore, we think that the present theoretical results of the SBH are applicable even to the doped systems, at least qualitatively.

Finally, we discuss the effects of the roughness of the interface structure. In the usual experiments on 6*H*-SiC(0001)/Ti (Refs. 2, 5, 6, 8, and 9) and 4*H*-SiC(0001)/Ti (Ref. 7) interfaces, the interface is not necessarily atomically flat, which means the existence of some steps, tilted regions, and rough regions in the interface. However, at least there should exist some coherent regions between disordered regions. And there exists the possibility that the SBH at such coherent regions consistent with our theoretical results should dominate the whole SBH of the interface. This may be the reason why our theoretical results of the SBH are consistent with usual experiments.[2,5–9]

E. Examination of the Schottky model

A dependence on the interface structure or interface species for SBH's obviously exists for the theoretical results of the 3*C*-SiC(111)/Ti and 3*C*-(001)/Ti interfaces[11] and for the experimental results of the 6*H*-SiC(0001)/Ti (Refs. 6 and 9) and 4*H*-SiC(0001)/Ti (Ref. 7) interfaces. However, the conventional SBH models such as the Schottky model and the MIGS-CNL model cannot explain this feature because these models deny such dependence as mentioned in Sec. I. As to the MIGS-CNL model, our calculated results indicate that the MIGS's have no significant effects on the SBH of the Si- and C-terminated 3*C*-SiC/Ti interfaces. The observed MIGS's seem to be tails of Ti states or tails of hybridization between dangling bonds and Ti orbitals, which are not similar to localized defect states to capture the carrier causing the Fermi level pinning.

On the other hand, recent experiments of the 6*H*-SiC(0001)/metal interfaces with reduced density of defects seem to indicate that the SBH behaves as a Schottky limit for various metals.[8,9] Thus, it is of interest to examine the applicability of the Schottky model to the present interfaces. Of course, in the original Schottky model, the work function (electron affinity) is regarded as the intrinsic constant for each material. Thus, this model cannot explain the difference in the SBH's for the Si- and C-terminated interfaces. However, the work function (electron affinity) depends seriously on the surface structure through the surface dipole caused by the charge distribution at the surface. Therefore, it is of great interest to examine the extended Schottky model dealing with such a realistic work function or an electron affinity. As mentioned above, we regard the SBH of the interface with no defects as the band discontinuity of the two materials dominated by two factors: the relation between the intrinsic band structures and the interface dipole. Similarly, the work function or the electron affinity is essentially the band discontinuity of the material/vacuum interface, which is also dominated by a similar two factors. Thus, examination of the extended Schottky model corresponds to examining whether the band discontinuity of the interface between the two materials can be estimated from the two kinds of band discontinuity of each material/vacuum interface or not.

In the present examination, we only consider the work functions of the Si- and C-terminated surfaces. The difference between the two surfaces corresponds to the difference in the SBH of the two interfaces in the extended Schottky model because of the common work function of the Ti surface. The theoretical work function is obtained as the difference between the vacuum level and the VBT of the bulk SiC region in *ab initio* calculations of the surface-slab supercell.[34] This is consistent with our theoretical definition of the *p*-type SBH. Note that we do not consider the positions of the surface states in the present case.

Figure 6 shows the averaged potential (AP) curves of (a) the relaxed (111) slabs and (b) the relaxed (001) slabs for both the Si- and C-terminated surfaces along the direction normal to the surface. The AP is the sum of the local component of pseudopotential, the Hartree potential, and the exchange-correlation potential averaged on each plane parallel to the surface. The nonlocal part of the pseudopotential existing only near atoms is neglected because of no long-range effects. The center of the AP in the bulk SiC region of each curve of the Si- or C-terminated surface is set to be equal to each other. Thus, we can get the difference in the work functions from the difference in the vacuum levels of the two curves, which corresponds to the difference in the *p*-type SBH in the extended Schottky model.

As seen in Fig. 6, the work functions of the C-terminated surface are larger than those of the Si-terminated ones in both the (111) and (001) slabs. This can be explained as follows. The amount of electrons outside of the C-terminated surfaces is larger than that of the Si-terminated one, because the C atom plays the role of anion in the SiC and has excess charge in comparison with the Si atom, which generates a large surface-dipole shifting of the electrostatic potential of the bulk region downward. The present results of the work functions mean that the *p*-type SBH's of the C-terminated (111) and (001) interfaces are larger than those of the Si-terminated (111) and (001) ones, respectively, in the extended Schottky model. This is contrary to our interface-supercell calculations and experiments. It is clear that the

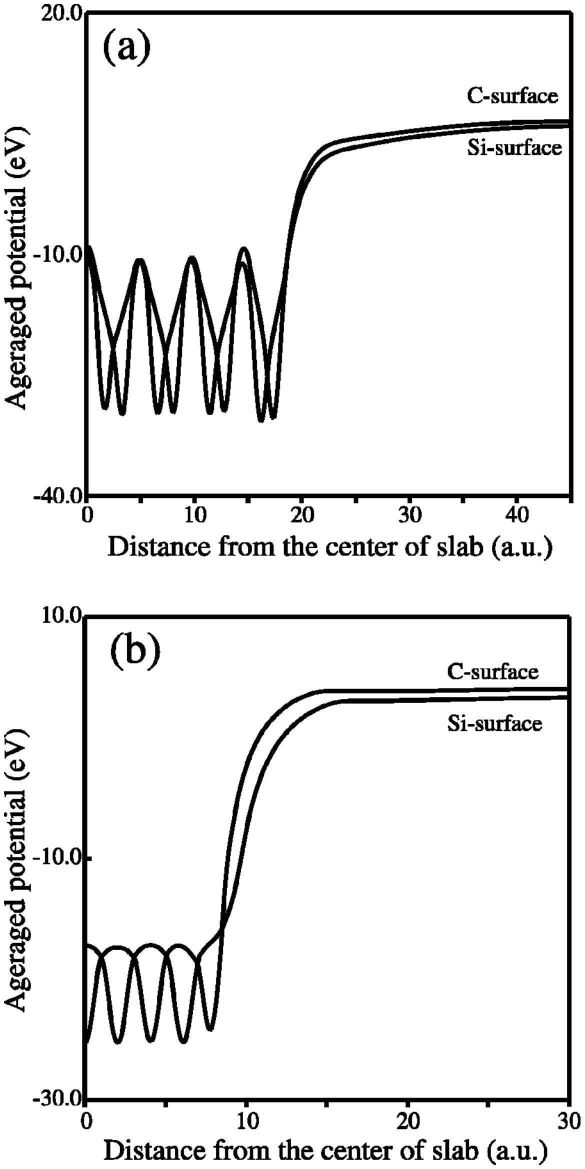

FIG. 6. Average potential profiles of (a) the relaxed (111) surface slabs and (b) (001) surface slabs along the ⟨111⟩ and ⟨001⟩ axes, respectively. Two types of surface slabs, SiC(Si) (Si surface) and SiC(C) (C surface), are shown. For each pair of the Si- and C-terminated surfaces, the center of the potential in the bulk region of the slab is set to be equal to each other. Thus, the difference in the vacuum levels of the two surfaces corresponds to the difference in the work function.

extended Schottky model cannot explain the SBH's of the Si- and C-terminated SiC/Ti interfaces. Thus, the interface property cannot be predicted correctly by the sum of the properties of two surfaces constituting interfaces. Consideration of practical interface structures should be essentially in order to analyze the SBH.

V. SUMMARY

The atomic and electronic structures of the 3*C*-SiC(111)/Ti polar interfaces are calculated by using the *ab initio* pseudopotential method. In stable configurations, the interfacial Ti atoms are located on top of the center of the triangle of the surface atoms of SiC(111) plane (T_4 site for the Si-terminated interface and H_3 site for the C-terminated one) rather than on top of the surface atoms (T_1 site). The stacking sequence of the Ti layers does not affect the total energy seriously in comparison with positions of the interfacial atoms. This point may be concerned with the experimental results that the fcc-Ti layers are generated on the atomically flat (0001) surface instead of the hcp-Ti.

In the stable configurations, the Si-Ti bond at the Si-terminated interface and the C-Ti bond at the C-terminated interface tend to have bond lengths similar to those in Ti silicide and TiC, although the lengths are somewhat larger than those in Ti silicide and TiC, respectively. The bonding nature of the Si-terminated interface reveals metallic and partial covalent character, while in the C-terminated one relatively strong covalent and ionic character can be seen. The adhesive energy of the C-terminated interface is larger than that of the Si-terminated one, which means that the former is stronger than the latter. In the LDOS of both the interfaces, there exist small peaks in the band gap of the LDOS of the SiC regions near the interface. These MIGS's almost disappear below the third layer inside SiC in both interfaces. It does not seem that such MIGS's have serious effects on the SBH of the present interface.

The *p*-type (*n*-type) SBH of the C-terminated interface is smaller (larger) than that of the Si-terminated one. This result is consistent with the experimentally observed difference of the SBH between the Si- and C-terminated 6*H*-SiC(0001)/Ti and 4*H*-SiC(0001)/Ti interfaces. This result can be understood by considering that the SBH is dominated by two factors: the relation of the intrinsic band structure and the interface dipole depending on the interface structures or species.

In comparison with the (001) interface, the bonding nature of the Si-Ti bond and the C-Ti bond at the Si- and C-terminated interfaces is basically similar to that in the (001) interfaces, and the SBH relationship between the Si- and C-terminated interfaces is also similar. However, the detailed features of the bond lengths, the bonding characters, the charge distribution, and the electronic structures are different. And especially the adhesive energy of the C-terminated (111) interface is smaller than that of the (001) interface, while the adhesive energy of the Si-terminated (111) interface is much larger than that of the (001) interface. These differences can be explained by the morphology of the interface structure depending on the interface plane such as the number of back bonds and neighboring atoms at the interface.

In comparison with the SiC(111)/TiC interface, the stable atomic configuration is similar to the present C-terminated interface, although the C atoms are inserted between the layers in the metal side. The relatively weak effect of the stacking sequence of the Ti layers on the total energy is also observed for the stacking of TiC layers in the SiC/TiC interface. The C-Ti distance of the C-terminated (111) interface is larger than that of the SiC/TiC interface because of the difference in the environment of the interfacial Ti atom. The *p*-type SBH of the C-terminated interface is smaller than that of the SiC/TiC one.

The extended Schottky model has been examined using the theoretical work functions of surfaces including the effects of surface structures. The calculated work function of the C-terminated surface is larger than that of the Si-terminated surface in both the (111) and (001) surfaces, which means that the *p*-type SBH of the C-terminated interface is larger than that of the Si-terminated one in the extended Schottky model. This is contrary to the SBH obtained by the supercell calculations of the interfaces and by experiments. It is clear that the interface properties are not able to be predicted correctly by the properties of surfaces constituting the interface.

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