

Ab initio calculations of the β -SiC(001)/Al interface

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The β -SiC/Al interface has been studied using the *ab initio* pseudopotential method, the conjugate-gradient technique proposed by Bylander, Kleinman, and Lee [Phys. Rev. B **42**, 1394 (1990)], and Troullier-Martins soft pseudopotentials [Phys. Rev. B **43**, 8861 (1991)]. Ionic and electronic structures at the interface, local density of states, Schottky-barrier heights, and bond adhesion between the two materials were determined for both the silicon-terminated and carbon-terminated interfaces. Results show a distinct difference between the Al-Si and the Al-C interactions effecting all aspects of the chemical bond, as well as bond adhesion. However, bond adhesion for both the Si-terminated and C-terminated interfaces is substantially greater than for nonreactive interfaces such as MgO/Al. [S0163-1829(98)10703-8]

I. INTRODUCTION

Due to the increasing application of metal-ceramic systems for electronic, structural, catalytic, and high-temperature applications, it is of great scientific interest to investigate the bonding nature and the origins of adhesion at metal-ceramic interfaces, where two solids of very different bonding characteristics are brought together.

Metal-ceramic interfaces can be classified into basically two categories: reactive and nonreactive.¹⁻³ For nonreactive systems, usually formed by ionic solids and noble or simple metals, it is assumed that the origin of adhesion is of a physisorption type, due to electrostatic effects such as image interaction and van der Waals forces. For reactive interfaces, formed from covalent ceramics and simple or transition metals, a chemisorption process with a large charge transfer and bond hybridization between the two materials is thought to occur. It is expected that bond adhesion for reactive interfaces is greater than for nonreactive interfaces and highly dependent on the configuration of atomic species.

Recently, *ab initio* calculations based on the density-functional theory have been applied to several metal-ceramic interfaces, although most of these studies have been confined to nonreactive systems. Calculations on the MgO/Ag (Refs. 3-5) and MgO/Al (Ref. 3) systems have confirmed that the origin of bonding between these solids is based on electrostatic effects, while the MgO/Ti (Ref. 6) system showed substantial orbital hybridization between the O 2*p* and Ti 3*d* orbitals. Al₂O₃/Nb (Ref. 7) interfaces have demonstrated rather strong ionic interactions between the O and Nb atoms, although interactions were dependent on surface stoichiometry.

For reactive interfaces, to date there have been only a few *ab initio* studies. The SiC/Al system itself has been studied previously by the use of tight-binding^{8,9} and cluster calculations;¹⁰ however, with these methods it is not possible to perform complete relaxations and at the same time allow for bond orbital hybridization, which is believed to be essential for an accurate description of such interfaces and is readily accomplished with the *ab initio* pseudopotential method. Therefore, in our previous study¹¹ *ab initio* pseudo-

potential calculations of the β -SiC(110)/Al were performed. In that study, a strong interaction between the C and Al atoms was found, exhibiting both covalent and ionic character and quite different from the Si-Al interaction. For our current study, a more detailed analysis has been performed, this time with the (001) interface, which allows for C-terminated and Si-terminated surfaces to fully distinguish between the C-Al and Si-Al interactions.

The need to understand the bonding nature of abrupt metal-ceramic interfaces has been demonstrated experimentally by recent techniques such as surface-activated bonding,¹² where microelectronic wafers can be bonded with clean, abrupt interfaces at room temperature without the production of reaction products. Many properties associated with these interfaces, such as the Schottky-barrier height,¹³ can play a determining role in the applicability of such materials when used as electrical devices such as light-emitting diodes. The *ab initio* pseudopotential method can provide insight into the bonding nature, bonding strength, and orientational preferences at an atomistic level that cannot be discerned through current microscopic techniques. Electronic properties such as local density of states, Schottky-barrier heights, and the origin of metal-induced gap states may also be investigated. For these reasons *ab initio* pseudopotential calculations are expected to be a valuable tool to investigate reactive metal-ceramic interfaces.

Our results show a vast difference between the carbon- and silicon-terminated interfaces in every facet of our study. This includes a difference in the Schottky-barrier height, helping to corroborate theories that correlate interfacial structure with this property. Metal-induced gap states (MIGS's) present in both Si-terminated and C-terminated interfaces differ greatly in their appearance and origin. The charge-density distribution at the interface, type of bonding between the two materials, and orientational preference of the Al layer over the two surfaces are also different and contribute to a bond strength for the C-terminated/Al bond that is much stronger than the Si-terminated/Al bond, although both bonds are stronger than for nonreactive interfaces. The details of our calculations and a discussion of our results follow.

TABLE I. Electronic configurations used for the calculation of pseudopotentials (local potential p) for C, Si, and Al.

Species and orbital	Occupation	Cutoff radius (a.u.)
C 2s	2.0	1.44
C 2p	2.0	1.44
Si 2s	2.0	1.8
Si 2p	0.5	1.8
Si 3d	0.5	1.8
Al 2s	1.0	1.8
Al 2p	0.5	2.0
Al 3d	0.5	2.0

II. CALCULATION METHOD

The SiC/Al system presents a number of problems when analysis of it is conducted with *ab initio* techniques. First is the fact that, unlike many of the studies of metal-ceramic systems involving metal-metal-oxide interfaces,³⁻⁷ the SiC/Al interface is a reactive one and due to the considerable time lengths involved with atomic migration, the study of a full interfacial reaction is currently time prohibitive for an *ab initio* simulation. However, as mentioned in the Introduction, abrupt, reaction-layer-free interfaces have also become technologically very important and *ab initio* calculations are well suited for this type of interface. Second, SiC and Al have a rather large equilibrium lattice mismatch ($\sim 8\%$), causing, as seen by electron microscopic techniques, periodic dislocations starting at the interface and continuing into the bulk regions.¹⁴ However, because of the rather stringent limitation on systems sizes (approximately 100 atoms) due to computer capacity and execution time, any system large enough to represent the full effect of lattice dislocations would be currently too large to study by *ab initio* methods. Thus only coherent interfaces can be represented. This, however, does not prevent study of the interactions of the interfacial species or further understanding of the bond nature between them.

For these purposes then the *ab initio* pseudopotential method using the conjugate-gradient technique proposed by Bylander, Kleinman, and Lee,¹⁵ with the Kerker mixing scheme,¹⁶ has been utilized to study the SiC/Al system. This method has been shown to be the most efficient for determining the minimum of the Kohn-Sham energy functional within the local-density approximation¹⁷⁻¹⁹ for large systems containing both metallic and ceramic bonding.¹¹ In order to reduce the number of required plane waves to describe the electron wave functions, Troullier-Martins-type²⁰ pseudopotentials in the fully separable Kleinman-Bylander²¹ form have been employed. Details of the electronic configurations used in constructing these pseudopotentials can be seen in Table I.

The simulation cells used to study the SiC/Al interface were chosen to both minimize computational time and required memory space while still providing an as accurate as possible representation of a real system. We deal with SiC(001) 1×1 ideal surfaces. For both the C-terminated and the Si-terminated supercells, a slab of nine (001) atomic layers was created, where both surfaces were terminated by the same species. Two sets of five Al(001) atomic layers were

then stacked upon these surfaces with the same two-dimensional 1×1 periodicity. Each (001) layer contains only one atom, for a total of 19 atoms in the supercell. These two identical interfaces were then separated by a vacuum region of approximately 15 a.u. to prevent an interaction between the two surfaces.

The SiC lattice constant was determined by minimizing the energy of a perfect SiC crystal using Troullier-Martins-type soft pseudopotentials, while varying the size of the unit cell. This lattice constant was determined to be 8.181 a.u., approximately 99.3% of the experimental value. However, since Al and SiC exhibit an equilibrium lattice size mismatch of $\sim 8\%$, the Al atoms were artificially placed in tension to form a coherent interface.

A plane-wave cutoff energy of 45 Ry was used, requiring 10 393 plane waves. This cutoff energy was arrived at by converging the total-energy calculations of each of the pure materials as a function of cutoff energy to 0.02 eV.

The initial configurations of the Al atoms over the SiC surfaces were set by translating the Al layers rigidly along the (001) plane. For the ideal 1×1 SiC(001) surface there exist four special positions that the Al atoms can occupy,⁸ corresponding to extrema on the energy surface, and give the total supercell a D_{2d} symmetry. These are the bridge site, the fourfold site, the on-top site over the surface atom, and the on-top site over the first atom below the surface. Each of these sites were tested to determine the lowest-energy position of the Al layers. For the Si-terminated surface, the Al atoms occupied the position of what would be the vacant carbon atoms in the SiC structure, thus maintaining the fourfold coordination of the Si atom. However, for the C-terminated system, the Al atoms were in their lowest-energy configuration when occupying the position directly above the surface carbon atoms in a cube-on-cube arrangement. The atoms were then relaxed by calculating the exact Hellmann-Feynman^{22,23} forces. The vacuum space between the two identical interfaces enabled a full relaxation of the Al and SiC layers; however, due to the symmetry of the system all atomic relaxations were along the z axis only and all x - y plane forces were equal to zero. After the relaxed positions of both the Si- and C-terminated surfaces of the SiC/Al interfaces were determined, the electronic structure, localized density of states, Schottky-barrier heights, and ideal work of adhesion were calculated. The electronic structure was determined on a real space grid of $32 \times 32 \times 256$ points, from ten special k points in the irreducible Brillouin zone. The eigenstates used in calculating the localized density of states were obtained from the ground-state charge-density data from this grid, using 23 k points in the irreducible Brillouin zone over 70 eigenstates. The Schottky-barrier height was measured from the Fermi level of the supercell systems to the top of the valence band of the bulk region of the SiC, determined by using the valence-band width of pure crystalline β -SiC. The ideal work of adhesion was calculated by comparing the total energy of the relaxed interfacial system with the total energy of the relaxed free surfaces of both SiC and Al.

III. RESULTS AND DISCUSSION

A. The carbon-terminated interface

For the C-terminated SiC surface, the lowest-energy position of the Al layer was directly above the C atoms, or a

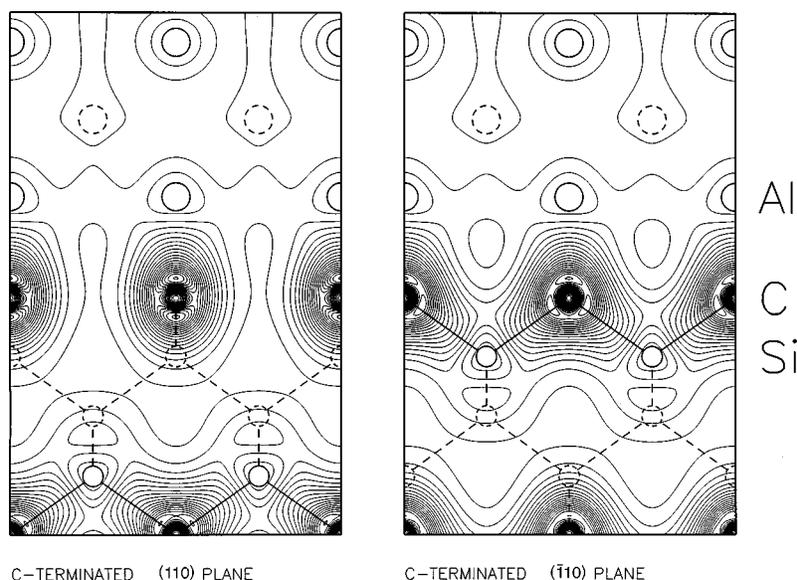


FIG. 1. Final relaxed ionic structure and charge density for the C-terminated SiC/Al supercell. Charge-density contours are from 0.001 to 0.301 a.u.⁻³ in spacings of 0.015 a.u.⁻³.

cube on cube arrangement. This causes the surface carbon atoms to be in a threefold-coordinated site, as opposed to the normal fourfold-coordinated sp^3 bonding of the bulk SiC. This signals either a more ioniclike bond between the C and Al interfacial atoms or an sp^2 orbital hybridization of the carbon atom. Both Figs. 1 and 2 indicate a charge transfer from the interfacial Al atom to the interfacial C atom. From Fig. 1 the ground-state charge density and atomic configurations of the C-terminated supercell can be seen. In this figure, as in all following figures, the small black spheres represent C atoms, large black spheres Si atoms, and gray spheres Al atoms. The C/Al interface has a very large electronic charge density between the interfacial atoms concentrated nearest the C atoms, while the charge density between the surface C and the second-layer Si atoms is slightly reduced from bulk levels.

The charge-density distribution, as taken along the z axis or the direction perpendicular to the interface, is shown in Fig. 2. Half the simulation cell is shown, or 128 grid points

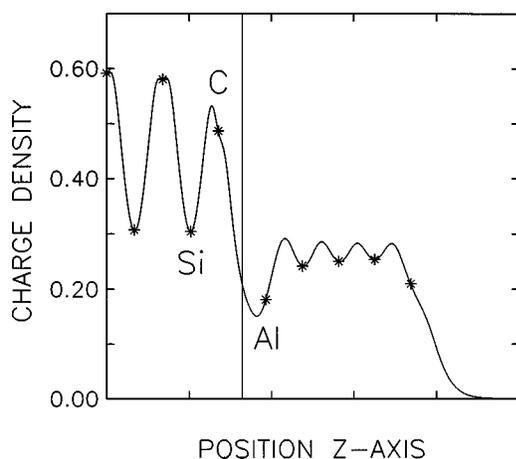


FIG. 2. Charge-density distribution for the C-terminated supercell along the z axis, as totaled in the x - y planes. The vertical line marks the interface between the Al and C layers.

of the total 256 z -direction grid points of the simulation cell, with the charge density totaled for every x - y grid point along the z direction. The distribution shows the depletion of the charge density near the interfacial Al atoms due to its bond with the C surface. The depletion of the charge density near the interfacial C from Fig. 2 is most likely due to the reduction in coordination of the surface atoms since the surface C atoms are only threefold coordinated. There is also a surface effect near the last Al atoms because of the vacuum space created in the simulation cell. The charge density within both the bulk Al and SiC seems relatively unaffected by the reaction at the interface.

The bond distances for the interfacial C atom with both its neighboring Si atoms and interfacial Al atom are virtually the same and the charge distribution around these three bonds are similar. This was also the case in our previous study of the SiC(110)/Al system, even though for the (110) system the interfacial C atom was four coordinated. This suggests a very similar covalent type of bonding for the surface-C-Al as is with the surface-C-Si bond and the threefold coordination suggests a possible sp^2 -type arrangement. To investigate whether this type of orbital hybridization is indeed occurring at the interface, the local density of states (LDOS) was calculated and shown in Fig. 3. The LDOS is calculated for each region between successive (001) atomic layers in the supercell. Dotted lines indicate the LDOS of the bulk SiC region of the supercell, although this has a slightly different shape than the DOS of the perfect SiC crystal. It is clear that the LDOS above the first layer of Al and below the first layer of Si recovers features very much like those of bulk Al and SiC DOS's. The LDOS's at the interface and the back Si-C bonds are substantially different from the bulk regions, both regions showing MIGS peaks that grow as one approaches the interface. This indicates that the Si-C back bonds have an electronic structure that is quite different from SiC bulk bonds and similar to the C-Al bonds, which supports the assumption of sp^2 -type bonding. Using the eigenvectors associated with these gap states, one can determine from which part of the supercell they are derived.

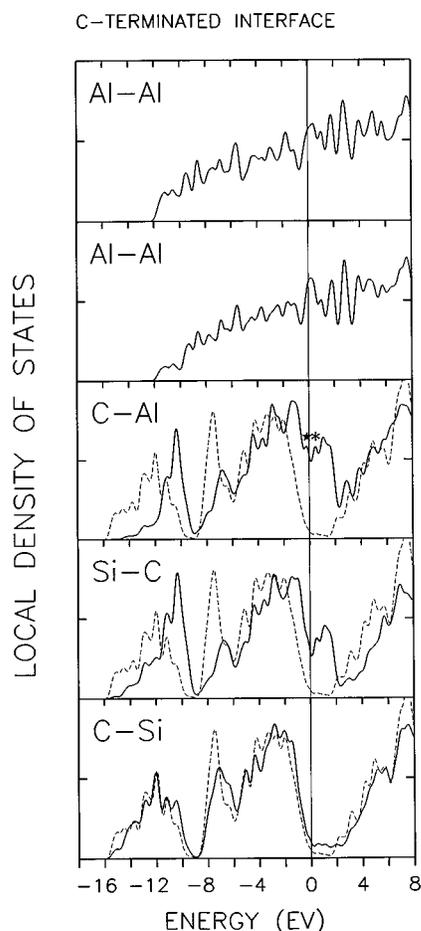


FIG. 3. Local density of states for the C-terminated supercell. The vertical line represents the Fermi energy.

Figure 4 shows the local charge density associated with the eigenvector at the Γ point for the peak labeled by a star in Fig. 3. This peak is an occupied state just below the Fermi level and appears to be a bonding p -orbital state between the interfacial C and Al atoms. It also has associated with it some surface Al charge. Figure 5, taken from the peak labeled with an asterisk in Fig. 3, appears to be a nonbonding p orbital in the $[100]$ direction, or perpendicular to the face of the paper, as seen in the figure, consistent with an sp^2 hybridization and one nonbonding p orbital of the interfacial C atom. A similar electronic structure of the surface C atom of an ideal 1×1 surface was observed in the tight-binding calculation by Hu *et al.*²⁴

B. The silicon-terminated surface

Figure 6 shows the final relaxed structure and ground-state electronic charge density of the Si-terminated (001) β -SiC/Al interface. As mentioned previously, for this interface the aluminum atoms at the interface sit in the position of what would be the vacant carbon atoms in the SiC structure. With the aluminum atoms in this position, the Si atoms at the interface maintains a fourfold coordination consistent with an sp^3 orbital hybridization. The charge between the surface Si atoms and the first Al atoms is relatively small and broadly distributed throughout the interfacial region, although there is a slightly greater density near the Si atom.

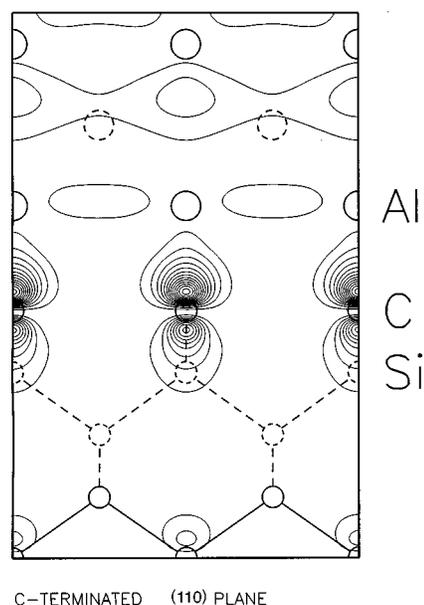


FIG. 4. Spatial representation of the eigenstate at the Γ point associated with the peak labeled with a star in Fig. 3. The bonding interfacial p orbital and Al surface charge effects are shown. Charge-density contours are from 0.001 to 0.0019 a.u.⁻³ in spacings of 0.000 15 a.u.⁻³.

This is similar to the charge density observed around the Si-Al bond in our previous study of the SiC(110)/Al system. The charge-density distribution, as totaled in the x - y planes along the z axis, is shown in Fig. 7. In this figure the charge transfer from the interfacial Al to the interfacial Si can be seen; however, it should be noted that the charge density of

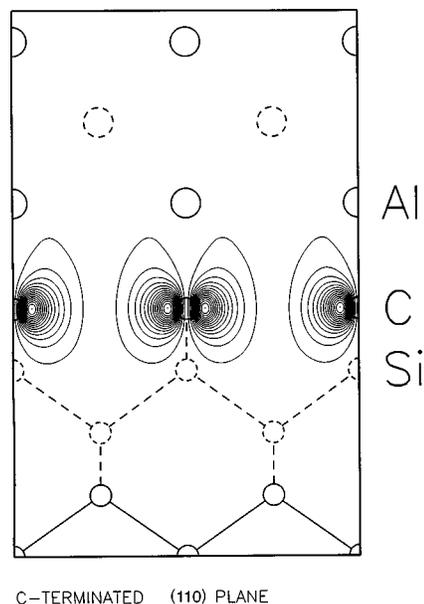


FIG. 5. Spatial representation of the eigenstate at the Γ point associated with the peak labeled with an asterisk in Fig. 3. The nonbonding interfacial p orbital aligned perpendicularly to the plane of the paper is shown. Charge-density contours are from 0.0005 to 0.018 a.u.⁻³ in spacings of 0.001 25 a.u.⁻³.

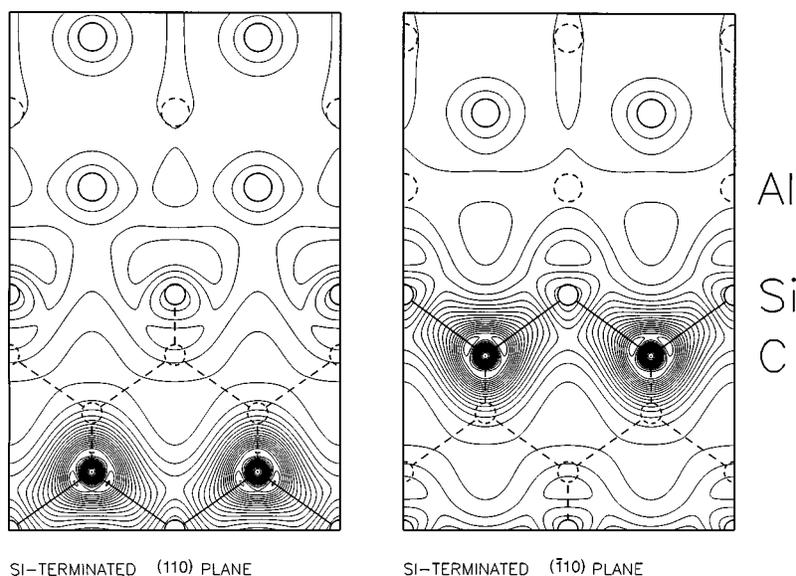


FIG. 6. Final relaxed ionic structure and charge density for the Si-terminated SiC/Al supercell. Charge-density contours are from 0.001 to 0.286 a.u.⁻³ in spacings of 0.015 a.u.⁻³.

the interfacial Al is very nearly the same value as that for the surface Al and only a very shallow depletion region is present near the interfacial Al. This is in contrast to the relatively large charge depletion around the interfacial Al when in contact with the C-terminated surface. The bond distance between the surface Si atoms and the interfacial Al atoms is much larger than the bond distances within the bulk SiC, 4.7 a.u vs 3.5 a.u., respectively. This is also much larger than the C-Al bond for the C-terminated case of 3.5 a.u.

The local density of states and the regions of the Si-terminated interface from where each graph is associated are shown in Fig. 8. As with the C-terminated supercell, metal-induced gap states appear near the metal-ceramic interface. However, unlike the C-terminated supercell, the density of states at the interfacial region itself has an appearance very similar to that of the metallic Al region instead of the bulk SiC region, suggesting a more metallic nature to the Si-Al bond. Also, the C-Si back bond seems to recover very quickly to features similar to the bulk SiC region. Examina-

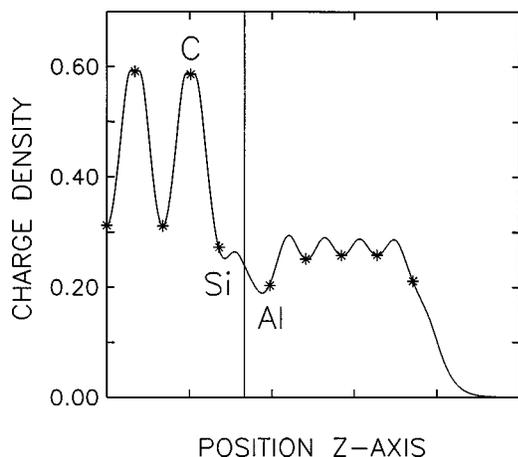


FIG. 7. Charge-density distribution for the Si-terminated supercell along the z axis, as totaled in the x - y planes. The vertical line marks the interface between the Al and Si layers.

tion of the charge densities associated with the metal-induced gap states show a broad distribution of charge in the interface region rather than a very localized charge density as was the case for the C/Al interface. Also, these gap states tend to involve the underlying carbon atoms as well as the

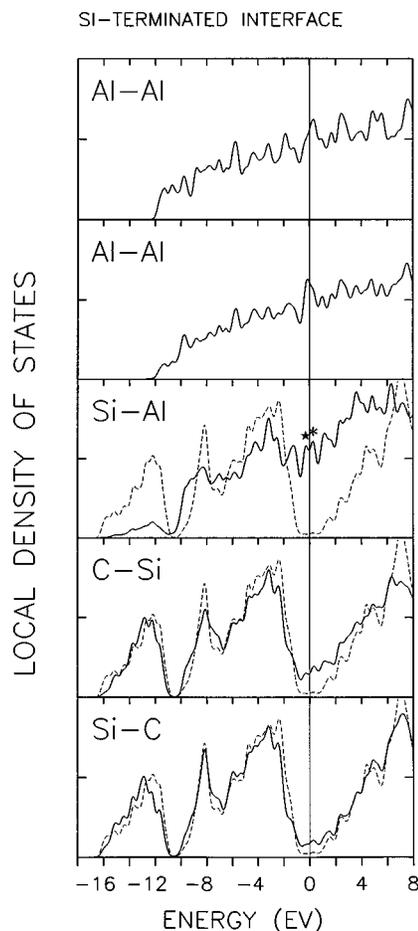


FIG. 8. Local density of states for the Si-terminated supercell. The vertical line represents the Fermi energy.

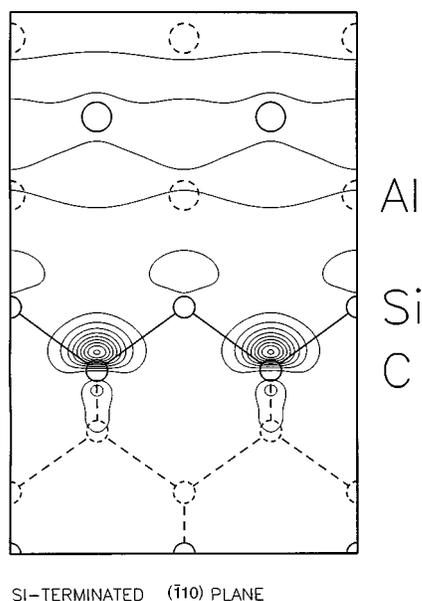


FIG. 9. Spatial representation of the eigenstate at the Γ point associated with the peak labeled with a star in Fig. 8. The participation in the creation of MIGS's is shared by both the Si surface and the underlying C atoms. Charge-density contours are from 0.0001 to 0.0013 a.u.⁻³ in spacings of 0.000 15 a.u.⁻³.

surface silicon atoms. Figure 9 shows the charge density associated with the eigenstate at the Γ point just below the Fermi energy and Fig. 10 for that which is associated with the eigenstate just above the Fermi energy, labeled with a star and an asterisk, respectively, in Fig. 8. These states contain the contribution from not only the Si p orbitals, but from C orbitals as well. It can be seen from these figures how the underlying C in the SiC plays an important role in creating

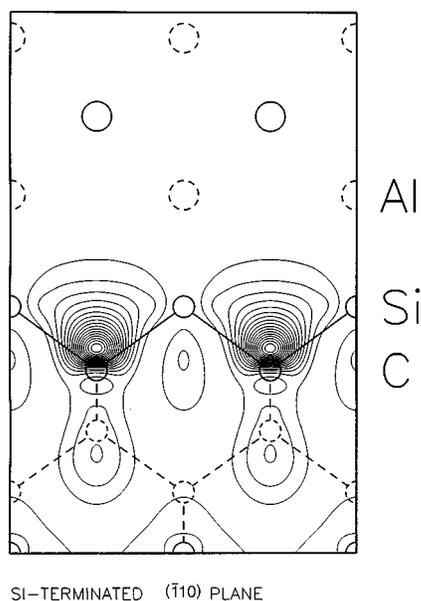


FIG. 10. Spatial representation of the eigenstate at the Γ point associated with the peak labeled with an asterisk in Fig. 8. The further contribution of the underlying C atoms to the MIGS's in the local density of states is shown. Charge-density contours are from 0.0001 to 0.0025 a.u.⁻³ in spacings of 0.000 15 a.u.⁻³.

TABLE II. Calculated bond adhesion of C- and Si-terminated supercells, pure aluminum surface energy, and work of adhesion for the Al/MgO system.

C-terminated supercell	Total energy (eV)
complete supercell	-1779.9
SiC only	-1203.2
Al only	-569.2
adhesion	6.42 (J m ⁻²)
Si-terminated supercell	Total energy (eV)
complete supercell	-1734.8
SiC only	-1161.2
adhesion	3.74 (J m ⁻²)
Pure aluminum	Adhesion energy
	2.04 (J m ⁻²) ^a
MgO/Al	Adhesion energy
	1.10 (J m ⁻²) ^a

^aReference 3.

these gap states. For the C-terminated case, no effect from the underlying Si was observed.

C. Bond adhesion

The bond adhesions for both the C- and Si-terminated interfaces were calculated by comparing the total energies of the relaxed interfacial systems with the total energies of the relaxed pure material surfaces without an interface and are shown in Table II. Although this method certainly does not produce the same quantitative results as an experimental test of a material, it can, however, be used as a qualitative comparison between the two different interfaces in this study.

For the C-terminated interface, the total energy of the full two-interface supercell was -1779.9 eV. For the C-terminated SiC 1×1 surface without the Al layer, the total energy was -1203.2 eV and for the Al 1×1 surface without the SiC layer, -569.2 eV. This resulted in a calculated bond adhesion of 0.401 eV/Å², or 6.42 J m⁻². The equivalent values for the Si-terminated interface were -1734.8 eV for the full supercell and -1161.2 eV for the SiC layer without the Al, resulting in a calculated bond adhesion of 0.234 eV/Å², or 3.74 J m⁻². From these results, it can be seen that the bonds between C and Al, having a more localized charge distribution at the interface, produce a bond almost twice as strong as the more dispersive Si-Al bond. These results can then be further compared to the ideal work of adhesion values obtained for the nonreactive MgO/Al interface, as calculated by Smith, Hong, and Srolovitz³ at 1.10 J m⁻², showing a bond strength of less than half that of the reactive SiC/Al interface, confirming the hypothesis that reactive metal-ceramic interfaces are quite large compared to nonreactive ones. In fact, with an adhesive energy of pure Al of only 2.04 J m⁻², as calculated by Smith, Hong, and Srolovitz,³ it is quite possible that the interfacial bond between the Al and SiC is stronger than the intralayer bonds within the pure aluminum.

TABLE III. Schottky-barrier heights ($E_F - E_{VB}$).

Property	Current study (eV)	Experiment (eV)
E_g of SiC (perfect crystal)	1.55	2.38
$E_F - E_{VB}$ C-terminated	0.08	
$E_F - E_{VB}$ Si-terminated	0.85	$\sim 0.9^a$

^aReference 32.

D. Schottky-barrier height

One very important property for determining the electrical and optical properties of devices that employ metal-ceramic interfaces is the Schottky-barrier height (SBH). In 1942, Schottky¹³ proposed his model relating the SBH to the difference between the metal work function and the electron affinity in the semiconductor. However, Heine²⁵ later stated that the pinning of the Fermi levels was due to MIGS's, which were caused by the tails of the metal wave functions decaying into the semiconductor. Louie and Cohen,²⁶ using local-density formalism, showed that indeed a high density of MIGS's is formed with the creation of a metal-ceramic interface. It was believed that the pinning position in the MIGS's was intrinsic to respective semiconductors. However, Tung, Gibson, and Poate²⁷ found experimentally that the SBH of a metal-ceramic interface is dependent on the interfacial structure, and these findings have been corroborated by the use of *ab initio* calculations based on the density-functional theory by Fujitani and Asano²⁸ and Das *et al.*²⁹ More recent *ab initio* calculations^{30,31} also indicate that the SBH is dependent on interfacial structure.

For the present system, the SBH for the C-terminated and Si-terminated SiC/Al interfaces have been calculated. Because of the rather poor estimation of the band-gap energy as calculated by using the local-density approximation, the SBH of a material simulated with this method is best defined as the difference between the Fermi level and the energy at the top of the valence band in the bulk SiC region ($E_F - E_{VB}$), which corresponds to the SBH of a *p*-type semiconductor, to avoid use of the highly inaccurate values for the excited states, and are best used only comparatively. However, the results (as shown in Table III) do show a definite interface structural dependence on the SBH, as has been found in the previous studies just eluded to, and actually agree quite well with the experimental findings for the Si-terminated surface.³² The energy gap (E_g) between the valence and conduction bands for the bulk SiC as calculated by the local-density approximation and the Troullier-Martins pseudopotentials used in this study was found to be 1.5 eV, as opposed to the experimental value of 2.38 eV. For the C-terminated supercell the SBH was found to be 0.08 eV and for the Si-terminated supercell 0.85 eV. This difference in the SBH can be clearly seen in the LDOS curves of Figs. 3 and 8. Experimentally, a value of 0.9 eV has been estimated for

$E_F - E_{VB}$ for Si-terminated surfaces,³² which agrees well with our findings. The dramatically smaller SBH of the C-terminated system is believed to be due to the interfacial dipole caused by the charge transfer from the Al layer to the interface C atoms as shown in Figs. 1 and 2. This dipole shifts the electrostatic potential of the Al layers downward, which is known to substantially effect the band discontinuity of two materials.^{33,34} Of course, the present interfaces con-

tain no interfacial defects as would normally occur in experiment and have been shown to effect SBH.³⁵ However, it is still very probable that the SBH of the C- and Si-terminated interfaces will prove to be quite different in experiment as well considering the very different bonding nature described above.

IV. SUMMARY AND CONCLUSIONS

In this study, the β -SiC(001)/Al interface was simulated using the *ab initio* pseudopotential method for the purposes of describing the bonding nature and strength of an abrupt metal-ceramic interface, calculating the value and providing insight into the mechanism behind the Schottky-barrier height, and contributing to the understanding of adhesion between metals and ceramics by expanding the study into the realm of the reactive metal-ceramic interface.

The results show a drastic difference between the Si-terminated and C-terminated surfaces as they are brought into contact with the Al layer. For the fully relaxed C-terminated supercell, the highly localized charge density at the interface, the amount of charge transfer from the Al layer to the C layer, and the equilibrium distance between Al and C atoms indicate a strong bond formation between the two layers. With the Si-terminated surface supercell this is not the case. A low, broadly dispersed charge density at the interface, large interatomic spacing between the Si and Al atoms, and small charge transfer are observed.

The observation of the LDOS of each supercell reveals that for the C-terminated case, the LDOS at the interface is very similar in form to that of the Si-C back bond, yet substantially different from the SiC bulk region or the Al bulk region, suggesting a unique bonding arrangement between the Si, C, and Al at the interface. However, for the Si-terminated case, the LDOS at the interface has a more metallic appearance, similar to that of the other Al layers, but the C-Si back bond returns rapidly to a bulk SiC-like appearance, suggesting a kind of bonding at the interface very different from that for the bulk SiC. Although both supercells exhibit MIGS's, analysis of the charge density associated with these states shows that for the C-terminated case, only the C-Al bonds are responsible in the creation of MIGS's and the underlying Si atoms play no part. However, with the Si-terminated case, the interfacial Si, as well as the underlying C, aids in the formation of MIGS's. These gap states also show a very localized, covalentlike bonding between the C and Al, consistent with an sp^2 orbital configuration, whereas for the Si/Al interface, a more dispersive, metalliclike bonding, though with some directionality, seems to be occurring.

As a result of these differences in bonding types between the two supercells, the magnitude of the bond strength and Schottky-barrier heights were also found to be quite dissimilar. For the C-terminated interface, the bond strength was found to be 6.42 J m^{-2} , compared to only 3.74 J m^{-2} for the Si-terminated interface. However, both of these values are high when compared to the strength of the bond between a nonreactive interface, such as MgO/Al, found to have a theoretical work of adhesion of approximately 1.10 J m^{-2} , or even when compared to the adhesive energy of pure Al itself, which is estimated to be 2.04 J m^{-2} . The Schottky-barrier height, as measured from the Fermi level to the top of the

valence band of the bulk region of the SiC, for the C-terminated and Si-terminated interfaces were 0.08 and 0.85 eV, respectively, providing evidence in support of an interface structural dependence on the Schottky-barrier heights of metal-semiconductor interfaces. This value for the Si-terminated SBH agrees well with an experimental estimate of 0.90 eV. The dramatically smaller C-terminated SBH is

thought to be the result of an interfacial dipole, shifting the electrostatic potential of the Al layer downward.

In conclusion, *ab initio* computer simulation has been shown to provide valuable insight into the nature of metal-ceramic interfaces. Of the SiC/Al interface in particular it has been shown that very different properties may result for this system depending on the surface species of the SiC when the interface is created.

- ¹M. W. Finnis, *J. Phys.: Condens. Matter* **8**, 5811 (1996).
- ²F. S. Ohuchi and M. Kohyama, *J. Am. Ceram. Soc.* **74**, 1163 (1991).
- ³J. R. Smith, Tao Hong, and D. J. Srolovitz, *Phys. Rev. Lett.* **72**, 4021 (1994).
- ⁴P. Blöchl, G. P. Das, H. F. Fischmeister, and U. Schonberger, in *Metal-Ceramic Interfaces*, edited by M. Ruhle, A. G. Evans, M. F. Ashby, and J. P. Hirth (Pergamon, Oxford, 1989), p. 9.
- ⁵Chun Li, Ruqian Wu, A. J. Freeman, and C. L. Fu, *Phys. Rev. B* **48**, 8317 (1993).
- ⁶U. Schonberger, O. K. Anderson, and M. Methfessel, *Acta Metall. Mater.* **40**, S1 (1992).
- ⁷C. Kruse, M. W. Finnis, V. Y. Milman, M. C. Payne, A. De Vita, and M. J. Gillan, *J. Am. Ceram. Soc.* **77**, 431 (1994).
- ⁸Lu Wenchang, Zhang Kaiming, and Xie Xide, *Phys. Rev. B* **45**, 11 048 (1991).
- ⁹Xiao Hu, Hong Yan, and F. S. Ohuchi, in *Diamond, SiC and Nitride Wide Bandgap Semiconductors*, edited by C. H. Carter, Jr., G. Gildenblat, S. Nakamura, and R. J. Nemanich, Materials Research Symposia Proceedings No. 336 (Materials Research Society, Pittsburgh, 1994), p. 15.
- ¹⁰S. Li, J. Arsenault, and P. Jena, *J. Appl. Phys.* **64**, 6246 (1988).
- ¹¹Masanori Kohyama, *Mod. Simul. Mater. Sci. Eng.* **4**, 397 (1996).
- ¹²T. Suga, in *Interface Science and Materials Interconnection*, edited by Y. Ishida (Japanese Institute of Metals, CITY, 1996), p. 13; H. L. Beck and F. S. Ohuchi, *ibid.* p. 45.
- ¹³W. Schottky, *Z. Phys.* **118**, 539 (1942).
- ¹⁴Toyohiko Yano, Satoshi Kato, and Takayoshi Iseki, *J. Am. Ceram. Soc.* **75**, 580 (1992).
- ¹⁵D. M. Bylander, Leonard Kleinman, and Seongbok Lee, *Phys. Rev. B* **42**, 1394 (1990).
- ¹⁶G. P. Kerker, *Phys. Rev. B* **23**, 3082 (1980).
- ¹⁷P. Hohenberg and W. Kohn, *Phys. Rev.* **136**, 864 (1964).
- ¹⁸W. Kohn and L. J. Sham, *Phys. Rev.* **140**, 1133 (1965).
- ¹⁹J. P. Perdew and A. Zunger, *Phys. Rev. B* **23**, 5048 (1981).
- ²⁰N. Troullier and José Luís Martins, *Phys. Rev. B* **43**, 8861 (1991).
- ²¹L. Kleinman and D. M. Bylander, *Phys. Rev. Lett.* **48**, 1425 (1982).
- ²²H. Hellmann, *Einführung in die Quantumchemie* (Deuticke, Leipzig, 1937).
- ²³R. P. Feynman, *Phys. Rev.* **56**, 340 (1939).
- ²⁴Xiao Hu, Hong Yan, Masanori Kohyama, and Fumio Ohuchi, *J. Phys.: Condens. Matter* **7**, 1069 (1995).
- ²⁵V. Heine, *Phys. Rev.* **138**, 1689 (1965).
- ²⁶S. G. Louie and M. L. Cohen, *Phys. Rev. B* **13**, 2461 (1976).
- ²⁷R. T. Tung, J. M. Gibson, and J. M. Poate, *Phys. Rev. Lett.* **50**, 429 (1983).
- ²⁸Hideaki Fujitani and Setsuro Asano, *Phys. Rev. B* **42**, 1696 (1990).
- ²⁹G. P. Das, P. Blöchl, O. K. Andersen, N. E. Chistensen, and O. Gunnarsson, *Phys. Rev. Lett.* **63**, 1168 (1989).
- ³⁰M. van Schilfgaarde and N. Newman, *Phys. Rev. Lett.* **65**, 2728 (1990).
- ³¹M. van Schilfgaarde, E. R. Weber, and N. Newman, *Phys. Rev. Lett.* **73**, 581 (1994).
- ³²V. M. Bermudez, *J. Appl. Phys.* **63**, 4951 (1987).
- ³³W. R. Lambrecht, B. Segall, and O. K. Andersen, *Phys. Rev. B* **41**, 2813 (1990).
- ³⁴W. R. Lambrecht and B. Segall, *Phys. Rev. B* **41**, 2832 (1990).
- ³⁵S. Hara, T. Teraji, H. Okushi, and K. Kajimura, *Appl. Surf. Sci.* **107**, 218 (1996).