Ab initio study of the Bi-covered GaAs(111)*B* surface

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An *ab initio* theoretical study has been performed, within the local-density approximation and the pseudopotential method, of the atomic geometry, electronic structure, and energetic stability of the Bi-covered GaAs(111)*B* surface. The results obtained support the stability of the $c(4\times2)$ reconstruction observed experimentally by McGinley *et al.* [Appl. Surf. Sci. **152**, 169 (1999)], for a Bi coverage of 0.75 monolayer, with the Bi trimers aligned along the $[11\bar{2}]$ direction. The Bi trimers are found to be energetically more favorable in the T_4 sites rather than in the H_3 sites. The electronic-band-structure calculations indicate that the surface is semiconducting in nature. The highest occupied surface state is resonant with the GaAs-bulk valence band, and is localized on the unbonded second-layer As atoms. The lowest unoccupied state is mainly localized on the Bi trimers, and exhibits a charge-density overlap between neighbor Bi trimers. In general, the electronic band structure, atomic geometry, and simulated scanning tunnel microscope images of the Bi-covered $c(4\times2)$ surface show similarities with the Sb-covered (3×8) and As-covered (2×2) surfaces.

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I. INTRODUCTION

A microscopic characterization of semiconductor surface reconstructions is fundamental to the development of electronic and optoelectronic devices. In particular, the stability and electronic structure of interfaces between different materials, forming heterojunctions, are strongly associated with the interface (or contact surface) properties. Recently, the study of the adsorption process, atomic topology, and electronic properties of the group-V covered III-V semiconductor surfaces have been the subject of many experimental and some theoretical studies. Extensive studies have been performed for an ordered deposition of group V on III-V(110) surfaces, with the conclusion that the adsorbates form chains and the surface generally remains unreconstructed[1] but in some cases exhibits a (2×1) reconstruction[2]. Deposition of Sb on GaAs(001)-$\beta2(2\times4)$ results in the surface reconstruction to change to (1×4), (1×3), and (2×4) phases in order of increasing annealing temperatures, with the (2×4) phase being characterized by the presence of a Sb-Sb dimer in the top layer and a As-As dimer in the third layer.[3] Deposition of group-V elements on anion-terminated III-V(111), viz. the III-V(111)B, surfaces has been reported to result in a large number of reconstructions, characterized by the formation of adsorbate trimers and chains (see, e.g. Refs. 4–6). Such surfaces have attracted special attention due to their piezoelectric effects.

Biegelsen *et al.*,[7] using scanning-tunneling-microscopy (STM) images and total-energy calculations, concluded the formation of adsorbate As trimers in the so-called T_4 sites on the (2×2) reconstructed GaAs(111)*B* surface. For this system 75% of the surface area is covered by adsorbate As trimers that are bonded to the surface As atoms, and on the remaining 25% surface area is exposed with the surface As atoms remaining nonbonded (these As atoms will be called "rest" atoms). The coverage of the adsorbate As atoms is, therefore, 0.75 monolayer (ML). Recently Stezer *et al.*[8] have, using surface core-level spectroscopy (SCLS), determined the atomic geometry of the As trimers on the GaAs(111)*B*-(2×2) surface. The Sb-covered GaAs(111)*B* surface has been extensively studied by Moriarty *et al.*[4–6] and Cafolla *et al.*,[9] using a number of different experimental approaches. These studies proposed a family of surface reconstructions, constrained to the electron counting rule (ECR), and the STM images suggested predominatly the (3×8) model, formed by Sb trimers (adsorbed in the T_4 sites) and Sb chains along the $[\bar{1}10]$ direction with Sb concentration of 0.75 ML (top layer) and 0.25 ML of As rest atoms (second layer). In addition, these studies have also concluded that an annealing process (at 475 °C) gives rise to a structural phase transition from the (3×8) to the (1×3) reconstruction. The latter model is formed only by Sb chains, but does not satisfy the ECR. Very recent theoretical studies have supported these experimental findings and explain that the stability of the (1×3) model comes from a strain-relieving mechanism.[10,11]

The Bi-covered GaAs(111)*B* surface has been studied by McGinley *et al.*,[12] using the SCLS and low-energy electron diffraction (LEED) techniques. Their work clearly indicates the formation of Bi trimers, a situation similar to the adsorption of some other group-V elements on the GaAs(111)*B* surface. However, whereas the As-covered GaAs(111) surface exhibits the (2×2) reconstruction,[7] and the Sb-covered GaAs(111)*B* surface exhibits the (3×8) and (1×3) reconstructions,[4–6] the Bi-covered GaAs(111)*B* surface exhibits (2×2) and $c(4\times2)$ reconstructions (below 110 °C and above 350 °C, respectively). A Bi-chain model is not compatible with the (2×2) and $c(4\times2)$ reconstructions, lending support to a Bi trimer model. In the $c(4\times2)$ model the Bi trimers are alternately shifted by $a\sqrt{2}/2$ ($a=$ lattice constant), along the $[\bar{1}10]$ direction, forming lines of Bi tri-

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mers along the $[11\bar{2}]$ direction. The adsorbate Bi atoms are bonded to 75% of the surface As atoms, while the remaining 25% surface As atoms remain exposed (called the As rest atoms). While the formation of group-V trimers (in T_4 sites) on the GaAs(111)B surface seems to be a common feature of these structures, it is remarkable that the formation of different types of surface reconstructions have been observed for different adsorbates.

While theoretical studies of the As- and Sb-covered GaAs(111)B surfaces have supported the experimental investigations, no theoretical studies are available on the Bi-covered system. In this work we present an *ab initio* study of the Bi-covered GaAs(111)B surface. The equilibrium atomic geometry and the stability of the experimentally proposed Bi/GaAs(111)B-$c(4\times2)$ reconstruction have been determined, the electronic band structure has been studied in detail, and STM images of occupied and unoccupied states have been simulated. To examine the dependence of electronic states on the arrangement of the Bi trimers, we have also calculated the band structure of the (2×2) structure. We have further provided a discussion on the similarities and differences of the $c(4\times2)$ system with the As- and Sb-covered GaAs(111)B surfaces.

II. METHOD

Our calculations were performed in the framework of the density functional theory,[13] within the local-density approximation using the Ceperley-Alder correlation[14] as parametrized by Perdew and Zunger.[15] The electron-ion interaction was treated by using norm-conserving, *ab initio*, fully separable pseudopotentials.[16] The wave functions were expanded in a plane wave basis set with a kinetic energy cutoff of 12 Ry. Increasing the energy cutoff to 16 Ry did not result in any appreciable change in the atomic geometry and the total energy calculations for the Bi-covered GaAs(111)B system, indicating that the basis set with the 12 Ry cutoff is totally adequate for the present study. The theoretical equilibrium lattice constant of 5.62 Å was used for bulk GaAs. In order to simulate the surfaces we used the repeatead slab method,[13] with a supercell containing six atomic layers and a vacuum region equivalent to twice the bulk lattice constant of the respective compound. To avoid the artificial electrostatic field, which arises from the application of the periodic boundary condition to the polar slab, we used a dipole correction.[17,18] A layer of fractionally charged hydrogen atoms was used to saturate the cation dangling bonds at the botton layer of the slab. The application of the pseudohydrogenated method in conjuction with the dipole-correction scheme has been shown to eliminate the presence of the microscopic electric field extending over the supercell containing the polar slab used in this work.[19] The electronic charge density was calculated using a set of four special k points in the irreducible part of the surface Brillouin zone. The four topmost layers were fully relaxed to within a force convergence criterion of 25 meV/Å.

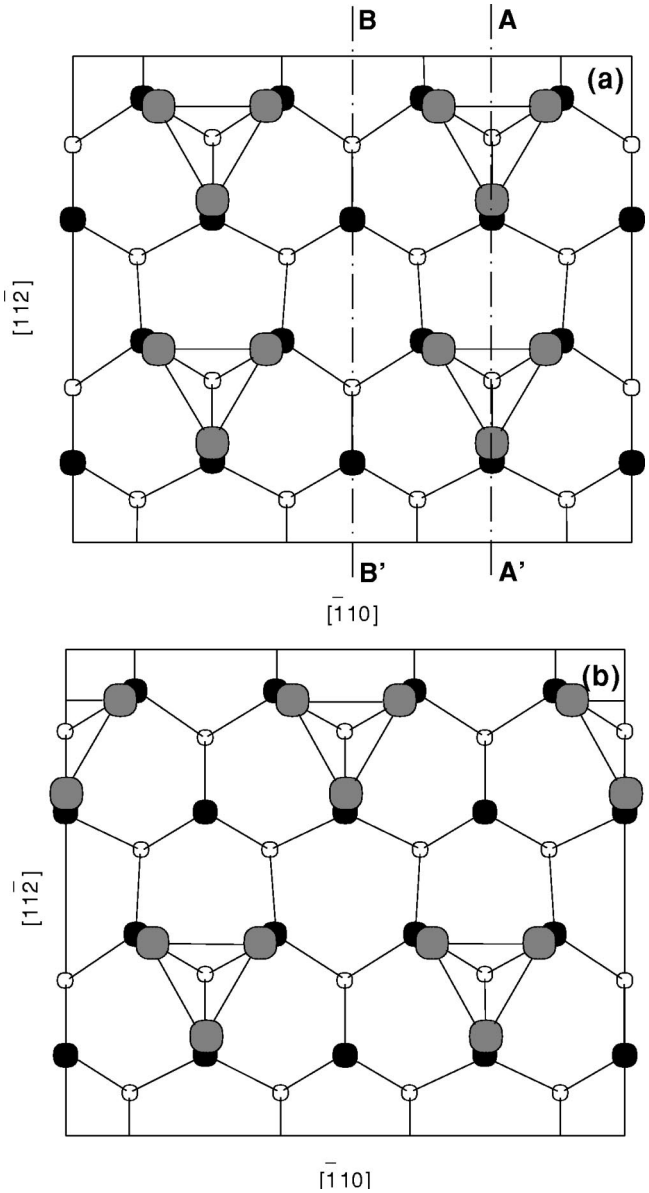

FIG. 1. Schematic top view of the atomic configurations of the Bi-covered GaAs(111)B surface within the (a) $c(4\times2)$ and (b) (2×2) models. The gray, black, and open cicles represent the Bi, As, and Ga atoms, respectively.

III. RESULTS AND DISCUSSIONS

The structural models of the Bi/GaAs(111)B-$c(4\times2)$ and Bi/GaAs(111)B-(2×2) surfaces are shown in Fig. 1, hereafter referred as to the $c(4\times2)$ and (2×2) models, respectively. The $c(4\times2)$ structure contains two Bi trimers per unit cell adsorbed in the T_4 sites (aligned along the $[11\bar{2}]$ direction) and two As rest atoms (forming a line of the As rest atoms parallel to the Bi trimers). In the equilibrium configuration the bond length between Bi atoms on the trimers is 3.07 Å, which is quite close to the bond length of Bi in the solid crystalline phase (3.10 Å in the rhombohedral structure). The bond length between the top-layer Bi adatom and the second-layer As atom is 2.73 Å, which is slightly bigger than the sum of the covalent radii of Bi and As atoms

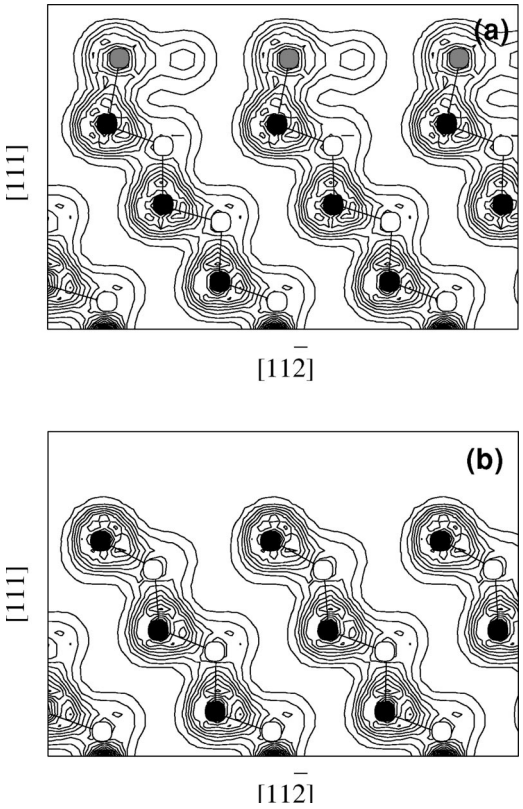

FIG. 2. Total charge density of the $c(4\times2)$ surface passing through the planes: (a) *A-A'* (containig the Bi trimers) and (b) *B-B'* (containing As rest atoms), as indicated in Fig. 1(a). The gray, black, and open cicles represent the Bi, As, and Ga atoms, respectively.

(2.67 Å), and the vertical distance (along the [111] direction) is 2.68 Å. Figure 2 presents the total charge density of the $c(4\times2)$ surface. The formation of the covalent bonds between Bi (top layer) and As (second layer) atoms is evident from Fig. 2(a). The As rest atoms are displaced vertically upward from the surface by 0.35 Å, resulting in a vertical distance between the As rest atoms and the third-layer Ga atoms of 1.16 Å. However, the As-Ga bond length is 2.43 Å, which is equal to the GaAs-bulk bond length. The total-charge-density plot in Fig. 2(b) shows the covalent bonding of an As rest atom with its neighboring Ga atom. The Ga-As bonds between Ga third layer and As fourth layer, below the Bi trimers, are compressed by 0.03 Å relative to the GaAs-bulk bond length (2.43 Å), resulting in a slight strengthening of these bonds.

In the (2×2) model, Fig. 1(b), the Bi trimers are also adsorbed in T_4 sites. Our calculations indicate that the equilibrium atomic geometry of this surface are almost identical to that of the $c(4\times2)$ surface. The bond length between the Bi trimer adatoms is 3.06 Å, and the vertical distance, along the [111] direction, between Bi (top layer) and As (second layer) is 2.68 Å. The vertical distance between As rest atoms and the third-layer Ga atoms is 1.19 Å, and the GaAs bonds between the Ga (third layer) and As (fourth layer) atoms, below the Bi trimers, are also compressed by 0.03 Å. Similar observations have also been made for the atomic geometry of the Sb-covered GaAs(111)B surface: (i) the As rest atoms are vertically displaced upward by 0.33 Å, and (ii) below the Sb trimers, the GaAs bonds are compressed by 0.05 Å relative to the GaAs bulk, and the bonds between the top-layer Sb adatoms and the second-layer As atoms are covalent.[10,11]

In order to examine the stable geometry of the $c(4\times2)$ model, we have studied a number of different atomic configurations for the Bi trimers on the GaAs(111)B surface. Initially we considered the adsorption of Bi trimers in the T_4 and H_3 sites. In both adsorption sites the atomic geometry of the Bi trimers are found to be very similar. However, our total-energy calculations indicate that the trimer adsorption in the T_4 sites is energetically more favorable than the adsorption in the H_3 sites, by 0.12 eV/trimer. A similar result has been verified by Biegelsen *et al.*,[7] for the adsorption of As trimers on the GaAs(111)B surface. In their work, the adsorption in the T_4 sites was found to be energetically more favorable by 0.06 eV/trimer. Recently, we have performed a total-energy calculation for Sb-trimers on the GaAs(111)B surface. Our results verify the conclusion reached by Biegelsen *et al.* and indicate that the Sb trimers in the T_4 sites is energetically more favorable by 0.11 eV/trimer.[10] From these results we establish a common charateristic for the adsorption process of group-V trimers on the GaAs(111)B surface: *the adsorption of the group*-V *trimers on the the* GaAs(111)B *surface is energetically more favourable in the* T_4 *sites than in the* H_3 *sites*.

Experimental observations suggest that the initial adsorption of Bi takes place at room temperature. The As trimers are substituted by the Bi trimers, retaining the (2×2) reconstruction of the clean GaAs(111)B surface [cf. Fig. 1(b)].[12] The coverage of Bi atoms is 0.75 ML, with 0.25 ML of As rest atoms. After an annealing process between 110 °C and 350 °C, LEED measurements indicate a structural transition from the (2×2) to the $c(4\times2)$ reconstruction on the Bi-covered GaAs(111)B surface. The annealing process beyond 300 °C allows for the maximum amount of Bi bonded to the surface. This is accomplished by shifting the adsorbed Bi trimers by $a\sqrt{2}/2$ along the [$\bar{1}\bar{1}$0] direction, thereby acquiring the $c(4\times2)$ structure [cf. Fig. 1(a)]. We have studied the relative stability of the $c(4\times2)$ and (2×2) models by comparing their total energies. To essure the same convergence criteria for these two models, the total-energy calculations were performed using the same 4×2 supercell. Our results indicate that the $c(4\times2)$ model is energetically more favourable than the (2×2) model by 0.06 eV/trimer (increasing the plane wave energy cutoff to 16 Ry, we obtained a total energy difference of 0.05 eV/trimer). Thus our work supports the favorability of the $c(4\times2)$ reconstruction proposed by McGinley *et al.* This rather low energetic favorability of the $c(4\times2)$ structure may be considered to support the observation[9] that the transition from the (2×2) to the $c(4\times2)$ structure takes place over a large temperature range. As discussed earlier, there is very little difference in the structural parameters for the two structures. The two structures can basically be distinguished by different distribution of the Bi trimers and As rest atoms. The small energetic favorabil-

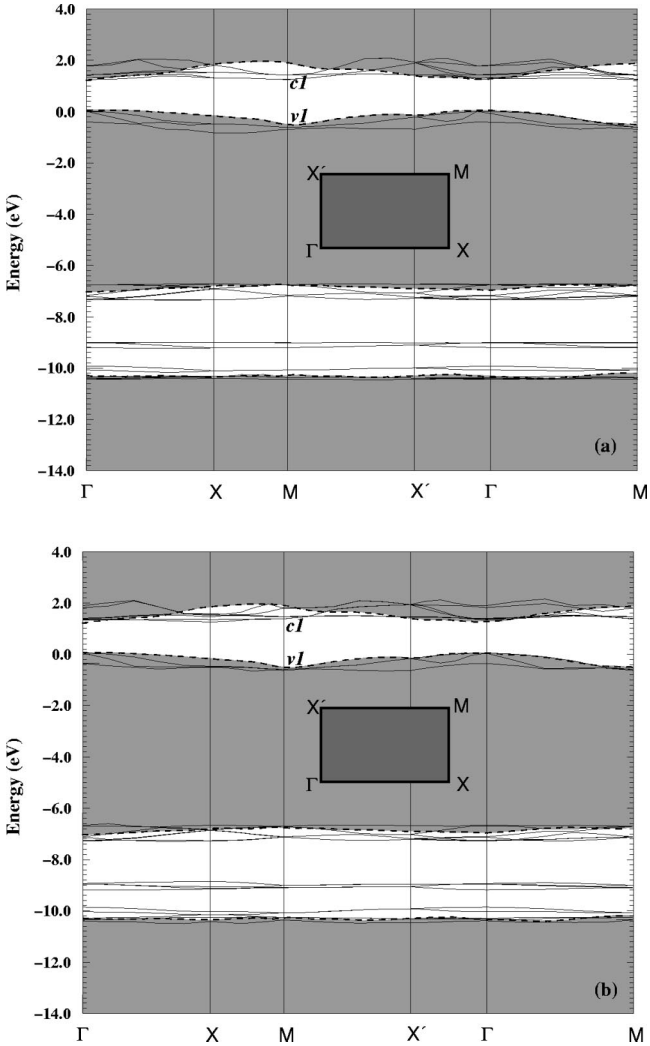

FIG. 3. Electronic band structure of the Bi-covered GaAs(111)B surface within the (a) (2×2) and (b) $c(4\times2)$ models. The solid lines indicate the surface states close to the fundamental and ionic gaps. The the shaded regions represent the GaAs-bulk projected band structure. The results for the (2×2) model are shown over the surface Brillouin zone for $c(4\times2)$, which is shown in the inset.

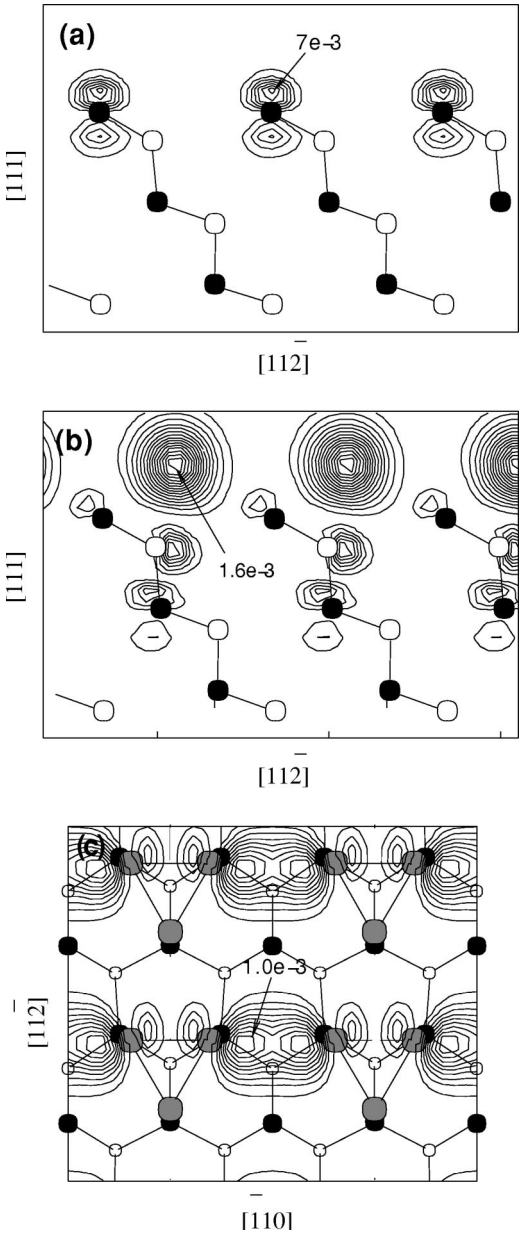

FIG. 4. Partial-charge-density plots for the Bi/GaAs(111)B-$c(4\times2)$ surface. Panel (a) shows the $v1$ state at the M point. Panels (b) and (c) show the side and top views, respectively, of the $c1$ state at the M point. Unit: electrons/(au)^3. The gray, black, and open cicles represent the Bi, As, and Ga atoms, respectively.

ity of the $c(4\times2)$ structure over the (2×2) structure is indicated by a slight overlap between the Bi trimers along a row for the former structure [cf. Fig. 5(c) and Fig. 5(d)). It is interesting to note that although the formation of trimers in the T_4 sites on the GaAs(111)B surface seems to be a common characteristic of the group-V adsorbate elements, the annealing process (at different temperatures) results in different atomic configurations on the surface: *the* (2×2) *reconstruction with trimer formation by* As *adsorbates; the* (3×8) *reconstruction with trimers and chains formed by* Sb *adsorbates; transformation of the* Sb-*induced* (3×8) *reconstruction into the* (1×3) *reconstruction after an annealing process at* 475 °C; *and the* $c(4\times2)$ *reconstruction with trimers aligned along the* $[11\bar{2}]$ *direction for* Bi *adsorption*.

Figure 3 shows the electronic band structure of the (2×2) and $c(4\times2)$ surface models. Our results indicate that these surfaces exhibit a very similar electronic band structure. Both models present a semiconducting character, keeping the fundamental band gap free of surface states. The similarity in the band structure for the two structures is consistent with their relative structural stability. The highest occupied surface state is resonant with the GaAs-bulk valence states. We also identified some surface states localized in the ionic gap, between 7 and 10 eV below the GaAs-bulk valence band maximum (VBM). The lowest unoccupied state is found to lie slightly above the GaAs-bulk conduction band minimum (CBM). Figure 4(a) shows the partial charge density plot of the highest occupied state ($v1$) at the M point.

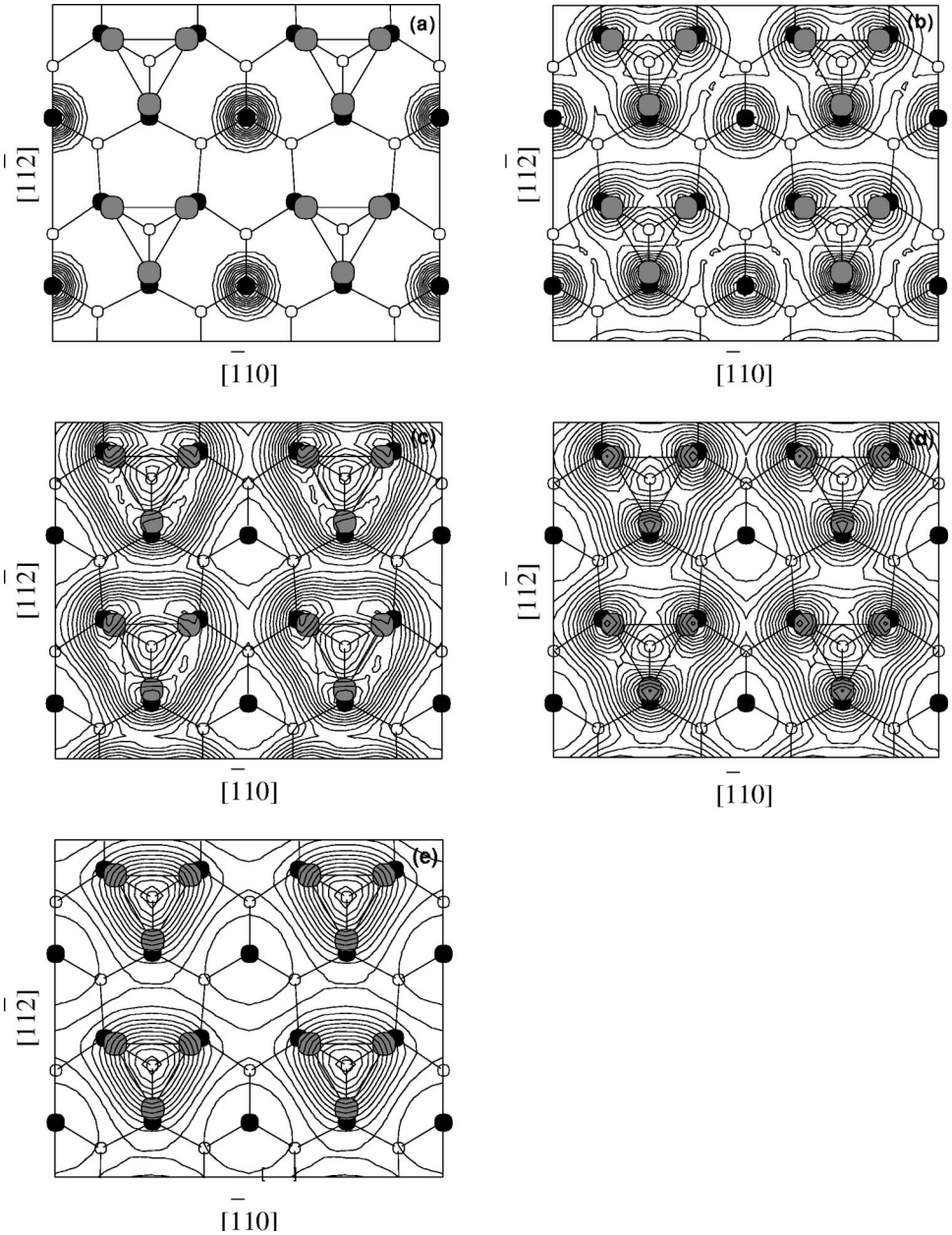

FIG. 5. Partial electronic charge density of the $c(4\times2)$ model at 1.22 Å above the second-layer As-rest atoms, for energy intervals of: (a) 0–1.5 eV, (b) 1.5–2.0 eV, below the calculated VBM, and at 2.43 Å above the top-layer Bi trimers, for for energy intervals of: (c) 0–1.5 eV, (d) 1.5–2.0 eV, below the calculated VBM, and (e) for unoccupied states for an energy interval of 1.0 eV above the calculated CBM. The gray, black, and open cicles represent the Bi, As, and Ga atoms, respectively.

Clearly this state arises due to the p_z orbitals localized on the As rest atoms. Figure 4(b) and Fig. 4(c) present the side and top views, respectively, of the partial charge density of the lowest unoccupied state ($c1$). This state is mainly localized on the Bi trimers, with a significant amount of orbital overlap between neighboring Bi trimers along the $[\bar{1}10]$ direction.

A general picture of the electronic structure of the $c(4\times2)$ model, which can be linked to the experimental STM observations, can be obtained by calculating the charge-density distribution for different energy windows in the valence and conduction bands. We have studied the partial charge density at 1.22 Å above the first-layer As rest atoms, and 2.43 Å above the adsorbate-layer Bi trimers. In Fig. 5(a) and Fig. 5(b) we present the partial charge density of the occupied states, within energy intervals of: 0–1.5 eV and 1.5–2.0 eV below the VBM (1.22 Å above the As rest atoms), respectively. Our results indicate that the highest occupied states, within an energy interval of 0–1.5 eV [Fig. 5(a)], are localized on the As rest atoms, with no contribution from the Bi-As backbonds. Between 1.5–2.0 eV [Fig. 5(b)] the charge density distribution is rearranged: while the charge is primarily localized on the As rest atoms, there is a significant amount of contribution from the Bi-As backbonds. For the energy interval 2.0–2.5 eV (not shown) the charge distribution is very similar to that for the energy interval 1.5–2.0 eV, but the charge density on the Bi-As backbonds has become more pronounced. Figure 5(c) and Fig. 5(d) present the partial charge density of the occupied states at 2.43 Å above the top-layer Bi trimers. For the energy interval 0–1.5 eV below the VBM [Fig. 5(c)], the involvement of the Bi trimers in covalent bond formation is clearly verified. However, at this distance from the surface, there is no contribution to the charge density from the As rest atoms. The charge localization on the Bi trimers becomes evident

for the energy interval 1.5–2.0 eV below the VBM [Fig. 5(d)], and this feature becomes more significant in energy interval 2.0–2.5 eV below the VBM (not shown). The density of states of the unoccupied orbitals at 2.43 Å above the top-layer Bi trimer, within an energy range of 1.0 eV above the CBM, is shown in Fig. 5(e). Our results indicate a high charge-density localization on the Bi trimers, with a protrusion on the trimers and a slight enlongation along the $[\bar{1}10]$ direction. This deformation can be attribuited to the charge-density overlap of the $c1$ state between different Bi trimers [see Fig. 4(c)]. The characteristics of the charge-density distribution on this surface, viz. (i) *charge localization of the highest occupied states on the first-layer* As *rest atoms and* (ii) *the charge localization of the lowest unoccupied state on the group*-V *trimers, have also been observed on the* Sb-*covered* GaAs(111)*B surface*.[10,11]

We have also performed a STM simulation of the $c(4\times2)$ surface within the Tersoff-Hamann approach.[20] To take into account the finite dimension of the real STM "tip," we have used the simulation procedure proposed by Lüdge *et al.*[21] and Miotto *et al.*,[22] by integrating the local density of states over a limited region above the surface top layer. In order to obtain images of occupied (unoccupied) states, we have summed the filled (empty) orbitals within different energy intervals below (above) the VBM (CBM). This procedure simulates the application of different values of the voltage to the sample with respect to the "tip." In our calculations the local density of states was calculated up to ≈ 4 Å above the Bi top layer. Figure 6(a) presents the result of the STM simulation for the occupied states, within an energy interval of 3.0 eV below the VBM. While the formation of Bi trimes has been clearly verified, with the maximum charge density being localized on the Bi atoms, the presence of the As rest atoms has not been observed, although as explained earlier the highest occupied states are mainly localized on the As rest atoms [cf. Figs. 4(a) and 5(a)]. In Fig. 6(b) we present the result of the STM simulation for the occupied states within an energy interval of 1.5 eV below the VBM. Similar to the Fig. 6(a), while the formation of the Bi trimers has been verified, the maximum charge density is localized along the Bi-Bi bonds. Even with the reduction of the "tip"-sample voltage, thus collecting only states near the VBM, the presence of the As rest atoms has not been observed. Our STM simulation, therefore, suggests that the STM images of the occupied states are representative of a picture of the surface topology, as previously commented by Kendrick *et al.*[23] in the experimental STM study of the In-terminated InAs(001) surface. Similarly, the simulated STM images of the Sb-covered GaAs(111)*B* surface, performed at constant current mode, are also closely related to the atomic topology of the surface, i.e., show Sb trimers and chains, with no infomation regarding the As rest atoms.[11] Figure 6(c) presents the STM image of the unoccupied states within an energy interval of 1.0 eV above the CBM. This image suggests a tunneling current into the empty dangling of the Bi trimers, but forming a central protrusion on the trimer region. These results are consistent with the previously obtained results for the partial charge-density distribution on the surface, as indicated in Fig. 5.

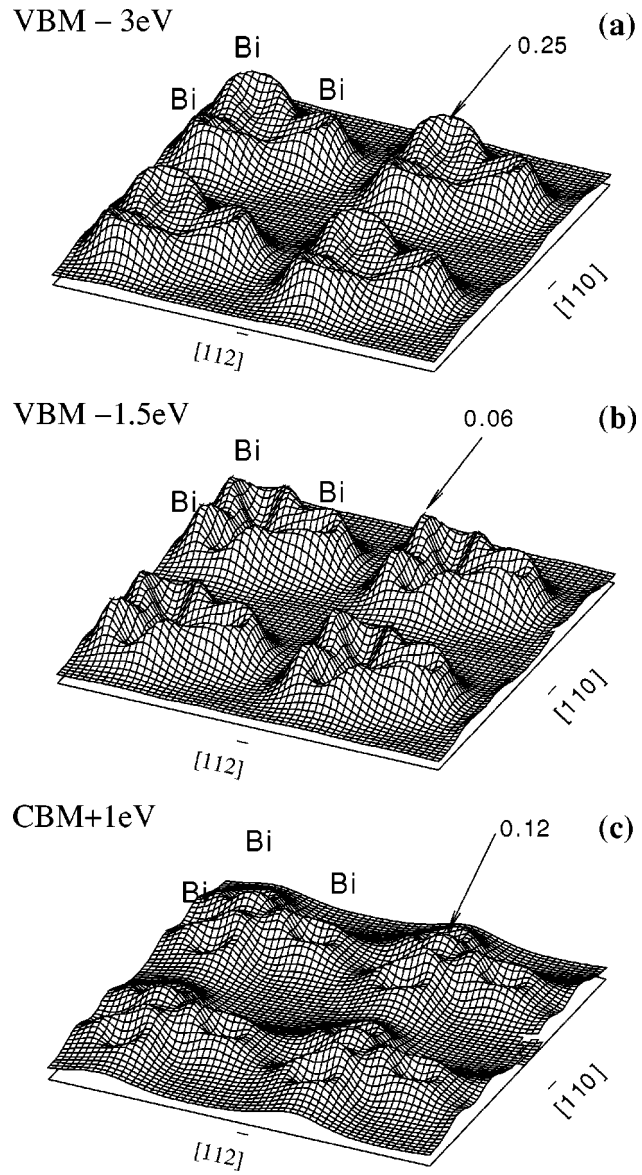

FIG. 6. STM images of the $c(4\times2)$ model for occupied states, for energy intervals of: (a) 3.0 eV and (b) 1.5 eV below the calculated VBM, and (c) for unoccupied states for an energy interval of 1.0 eV above the calculated CBM. Unit: electron/(au)^3.

IV. CONCLUSION

In conclusion, we have performed a detailed study of the atomic geometry, stability, and electronic structure of the Bi/GaAs(111)B-$c(4\times2)$ surface. Our results indicate that, in common with other group-V trimers, the Bi trimers are adsorbed in the T_4 sites. On the other hand, the atomic reconstruction of the Bi-covered GaAs(111)B surface is quite different from the As- and Sb-covered surfaces. Our total-energy calculations indicate that the $c(4\times2)$ model, with the Bi trimers aligned along the $[11\bar{2}]$ direction, is slightly more stable than the (2×2) model, supporting the recent experimental findings by McGinley *et al.* The surface equilibrium geometry for both the (2×2) and $c(4\times2)$ structures, including the presence of the As rest atoms, is very similar to that of the Sb/GaAs(111)B-(3×8) surface. The electronic

structure calculations indicate that both the (2×2) and the $c(4\times2)$ surfaces show a semiconducting character, with the highest occupied state being resonant with the GaAs valence band, and mainly localized on the unbonded As atoms. The lowest unoccupied state lies slightly above the GaAs-bulk conduction band minimum, and is characterized by a charge density that is asymmetrically distributed on the Bi trimers, with a significative charge-density overlap along the $[\bar{1}10]$ direction, i.e., between different trimers. The calculated charge-density distribution for the $c(4\times2)$ structure indicates that within an energy interval of 1.5 eV below the VBM the charge is localized on the first-layer As rest atoms. There is a significant amount of charge localization in the Bi-As backbonds in the energy interval of 1.5 eV below the VBM. In general, it is found that both the atomic equilibrium geometry and the electronic structure of the Bi/GaAs(111)-$c(4\times2)$ show similarities with the results for the Sb/GaAs(111)-(3×8) surface. The simulated STM images of the occupied states are strongly associated with the surface topology: the formation of Bi trimers has been clearly verified, and the STM images of the unoccupied states indicate the formation central protrusions localized on the Bi trimers. Similar results have been verified for the Sb-covered GaAs(111)B surface.

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[1] W.G. Schmidt, F. Bechstedt, and G.P. Srivastava, Surf. Sci. Rep. **25**, 141 (1996), and references therein.
[2] S.C.A. Gay and G.P. Srivastava, Phys. Rev. B **61**, 2688 (2000); and references therein.
[3] P. Moriarty, P.H. Beton, Y.-R. Ma, M. Henini, and D.A. Woolf, Phys. Rev. B **53**, 16 148 (1996); G.P. Srivastava and S.J. Jenkins, Surf. Sci. **377-379**, 23 (1997).
[4] P. Moriarty, P.H. Beton, and D.A. Woolf, Phys. Rev. B **51**, 7950 (1995).
[5] P. Moriarty, P.H. Beton, M. Henini, and D.A. Woolf, Surf. Sci. **365**, L663 (1996).
[6] P. Moriarty, P.H. Beton, and D.A. Woolf, J. Vac. Sci. Technol. B **B14**, 1024 (1996).
[7] D.K. Biegelsen, R.D. Bringans, J.E. Northrup, and L.-E. Swartz, Phys. Rev. Lett. **65**, 452 (1990).
[8] C. Setzer, J. PLaten, H. Bludau, M. Gierer, H. Over, and K. Jacobi, Surf. Sci. **402-404**, 782 (1998).
[9] A.A. Cafolla, C. McGinley, E. McLuoghlin, H. Hughes, P. Moriarty, A.W. Dunn, Y.-R. Ma, D. Teehan, B. Murphy, S. Downes, and W. Woolf, Surf. Sci. **377-379**, 130 (1997).
[10] R.H. Miwa and G.P. Srivastava, Surf. Sci. **482**, 1308 (2001).
[11] R.H. Miwa and G.P. Srivastava, Phys. Rev. B **63**, 125341 (2001).
[12] C. McGinley, A.A. Cafolla, B. Murphy, D. Teehan, and P. Moriarty, Appl. Surf. Sci. **152**, 169 (1999).
[13] G.P. Srivastava, *Theoretical Modelling of Semiconductor Surfaces* (World Scientific, Singapore, 1999).
[14] D.M. Ceperley and B.J. Alder, Phys. Rev. Lett. **45**, 566 (1980).
[15] J.P. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981).
[16] L. Kleinman and D.M. Bylander, Phys. Rev. Lett. **48**, 1425 (1982); X. Gonze, R. Stumpf and M. Scheffler, Phys. Rev. B **44**, 8503 (1991).
[17] J. Neugebauer and M. Scheffler, Phys. Rev. B **46**, 16 067 (1992).
[18] W.G. Schmidt, Appl. Phys. A **65**, 581 (1997).
[19] R.H. Miwa and G.P. Srivastava, Phys. Rev. B **62**, 15 778 (2000).
[20] J. Tersoff and D.R. Hamann, Phys. Rev. B **31**, 805 (1985).
[21] K. Lüdge, P. Vogt, O. Pulci, N. Esser, F. Bechstedt, and W. Richter, Phys. Rev. B **62**, 11 046 (2000).
[22] R. Miotto, G.P. Srivastava, and A.C. Ferraz, Phys. Rev. B **62**, 13 623 (2000).
[23] C. Kendrick, G. LeLay, and A. Kahn, Phys. Rev. B **54**, 17 877 (1996).