

# First-principles investigation of tip-surface interaction on a GaAs(110) surface: Implications for atomic force and scanning tunneling microscopies

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*Ab initio* pseudopotential total energy techniques are used to investigate the tip-surface interaction in atomic force microscopy on a GaAs(110) surface with a Si tip. Our simulations show significant surface relaxation effects in the near contact region, which lead to a complicated behavior of the total energy and force curves. In particular, the tip-induced displacement of the Ga atoms can exceed 1 Å even in the attractive force region, leading to hysteresis in the energy and force curves. These large tip-induced relaxations of the surface Ga atoms provide a natural explanation to the simultaneous imaging of both anions and cations in recent near-contact scanning tunneling microscopy experiments on this surface. We show that, for tip-surface distances where the surface topography remains unchanged and for a charge neutral Si tip, only the anion sublattice can be resolved in noncontact atomic force microscopy. Close to contact, our simulations prove that, even for atomically sharp tips (1) there is a significant contribution to the total interaction from tip atoms different from the apex atom; (2) large lateral (bonding) forces on the tip apex may develop and change the tip structure well before significant normal repulsive forces appear. [S0163-1829(99)09939-7]

## I. INTRODUCTION

The atomic force microscope (AFM) was developed as a technique for obtaining atomic-scale images of both conductors and insulators. In its constant force mode the surface structure is determined by measuring the variation of the tip height, which yields a constant (repulsive) force as the tip scans across the surface.

Compared with the scanning tunneling microscope (STM) the AFM probes atomic tip-surface interaction which, in principle, is more directly related to the surface atomic structure. However, in the constant force mode in most experiments on compound semiconductor surfaces such as GaAs(110),<sup>1</sup> InP(110),<sup>2</sup> InAs(110), and ZnSe(110),<sup>3</sup> neither atomic defects nor adsorbates were observed, while they are routinely observed with STM. The possible origin is thought to be the damage in the tip and in the substrate caused by the large repulsive forces ( $\sim$  several nN), although very little is actually known about the details of such processes.

The lack of true atomic resolution in the usual contact mode AFM has been solved by the use of dynamic force microscopy and a new operation mode, the frequency shift mode, probing the attractive force region. Recently Giessibl,<sup>4</sup> Kitamura and Iwatsuki,<sup>5</sup> and Ueyama *et al.*<sup>6</sup> have demonstrated that the AFM operating in this mode can give true atomic resolution.

In the frequency shift mode the tip oscillates with its eigen-frequency  $\omega$  and moves in and out of the interaction region during each oscillation cycle. Due to the tip-surface interaction, the new eigenfrequency is modified by  $\Delta\omega$  from the original eigenfrequency  $\omega_0$ .  $\Delta\omega$  is generally related to the energy ( $E$ ) and force ( $F$ ) of the tip-surface interaction. For the sake of convenience, here the quantity to which the  $\Delta\omega$  is proportional is denoted by  $X(E, F)$ . Therefore, a scan at a constant  $\Delta\omega$  will give an image that is a map of a constant  $X$ . Previously, it was thought that the quantity  $X$  should be the force gradient, and therefore an AFM image should be a map of the constant force gradient. Although this concept has been adopted broadly in recent literature,<sup>7-10</sup> it does not have a sound basis. Very recently, a careful numerical analysis of a Si tip interacting with the Si(111) surface showed that the quantity  $X$  is not the force gradient but is, to a good approximation, the geometric mean of the force and the potential energy<sup>11</sup> for typical experimental conditions.<sup>12,13</sup>

The physical origin of the contrast observed in these non-contact AFM images is far from clearly understood. For example, the contrast of the AFM image of Si(111)- $7\times 7$  surface does not seem to reflect the real topography of the surface and is affected remarkably by the tip material.<sup>7,14,15</sup> The non-contact AFM images have also been carried out for

InP(110), GaAs(110), and InAs(110) surfaces,<sup>8,16,17</sup> but usually the two sublattices could not be resolved in the images. All these questions are very closely related to the characteristics of the tip-surface interaction and the relaxation effects taking place both at the tip and the surface, which have not been well characterized so far. Theoretical simulations provide an effective tool to address the aforementioned questions.

In this paper, we report systematic *ab initio* calculations of the tip-surface interaction between a Si tip and a GaAs(110) surface. This surface has distinctive features, which make its imaging much more challenging than the case of the Si(111)- $7\times 7$  reconstruction, where most of the experiments were done so far. The (110) surface of the III-V compounds retains the  $1\times 1$  symmetry of the ideal surface, but the two atoms in the unit cell undergo important relaxations in the direction normal to the surface: The group-V atom (anion) moves outwards, while the III-group atom (cation) moves inwards. The driving mechanism for this atomic rearrangement is that it allows the cation (anion) surface atoms to adopt a  $sp^2$ -like ( $p$ -like) bonding configuration with its three neighbors, close to the planar (pyramidal) configuration of the  $\text{GaH}_3$  and  $\text{AsH}_3$  molecules, that lowers the total energy of the system. This relaxation has an important effect on the electronic levels in the energy gap, pushing the dangling bond related states of the anion towards the valence band and making them to be doubly occupied, and the ones related to the cation to the conduction band, leaving them empty. Furthermore, the relaxation decreases the stability of the surface atoms towards relaxations induced by dangling-bond-type interactions between the tip and the surface compared with the situation for the adatoms/rest atoms on the Si(111)- $7\times 7$  reconstructed surface. Hence, we expect the tip-induced surface relaxation effects to be much more important on the (110) surface. On the other hand, as the surface retains the  $1\times 1$  periodicity, the lateral distance between surface atoms is much smaller than in the case of the adatoms on the  $7\times 7$ , which favors the presence of multiple bonding interactions between the atoms on the tip and the surface in the near contact regime, even for sharp tips such as those considered here.

In this paper, we focus our attention on two questions. First, we characterize the tip-induced relaxation effects taking place when we approach the tip and the surface, and analyze its consequences for the total energy and force curves, whose shape deviates significantly from the results obtained in the theoretical study of the Si(111)- $5\times 5$  surface.<sup>9,10</sup> Secondly, we discuss the conditions for the simultaneous imaging by noncontact AFM of both the anion and cation sublattices on the surface. The large tip-induced relaxation effects found in our simulations also provide a natural explanation for some recent near-contact STM experiments on GaAs(110) surfaces, where both the anions and cations were simultaneously imaged. The present paper is complementary to the paper by Tóbiš *et al.*<sup>18</sup> on the InP(110) surface. We show that, in spite similarities between the experimental AFM images of the two surfaces, the potential energy surface sampled by the Si tip on the two surfaces exhibits striking differences in the near surface region.

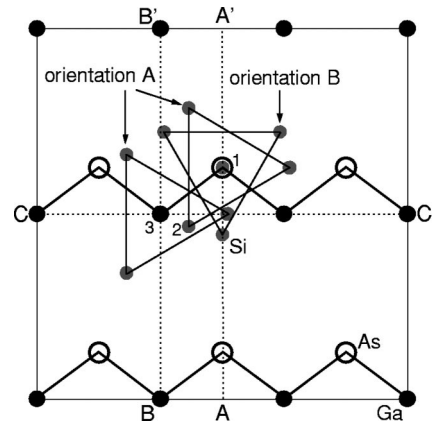


FIG. 1. Top view of the supercell used (unrelaxed). The white circles correspond to the As atoms and the black ones to Ga. The tip is represented by four hatched solid circles, the H atoms attached on the base layer of the tip are not shown. Two orientations (*A* and *B*) of the tip are considered when the tip scans vertically on top of the As atom denoted by “1.” The paths along which the tip performs lateral scans are denoted by the dotted lines.

## II. COMPUTATIONAL DETAILS

We have considered a supercell that contains a GaAs(110) slab and a Si tip. The slab has a  $2\times 3$  in-plane size and consists of seven layers in the normal direction. We consider a tip, which consists of four Si atoms with the three base Si atoms saturated by nine H atoms. Such a tip was first used by Pérez *et al.*<sup>9,10</sup> They showed that the saturation of the dangling bonds on the Si atoms on the tip base changes the hybridization of the apex atom, leaving one dangling bond pointing from the apex atom towards the surface. They also compared the total energy and forces obtained with a 4-Si-atom and a 10-Si-atom tip having otherwise the same tetrahedral structure and showed that the interaction is dominated by the apex dangling bond. Hence, the use of the 4-Si-atom tip for the purpose of this paper is justified.

The relaxed geometries were obtained by switching on the interaction between a separately relaxed surface and tip structure and relaxing the interacting system. The comparison of our relaxed surface with the ideal surface structure shows that the As atoms move upwards and the Ga atoms move downwards, leading to a surface buckling of 0.70 Å. This value is in good agreement with other theoretical calculations.<sup>19</sup> The separation between the tip base and the other surface of the slab is kept larger than 12.1 Å. The total size of the supercell, which contains 97 atoms, is 12.0 Å  $\times$  11.3 Å  $\times$  32.0 Å (equivalent to about 200 bulk atoms). The top and side views of the supercell are shown in Figs. 1 and 2, respectively. In order to explore the effect of multiple bonding interactions among the atoms in the tip and the surface, two different orientations of the tip with respect to the symmetry directions of the surface unit cell, shown in Fig. 1, have been considered.

The energies and atomic forces were calculated in the framework of density-functional theory in its plane-wave pseudopotential formulation.<sup>20</sup> In all the calculations the electronic orbitals were expanded at the  $\Gamma$  point of the Brillouin zone with a cutoff energy of 9 Ry. Optimized Troullier-Martins-type pseudopotentials were used for the atomic cores and the PW91 version<sup>21</sup> of generalized gradient

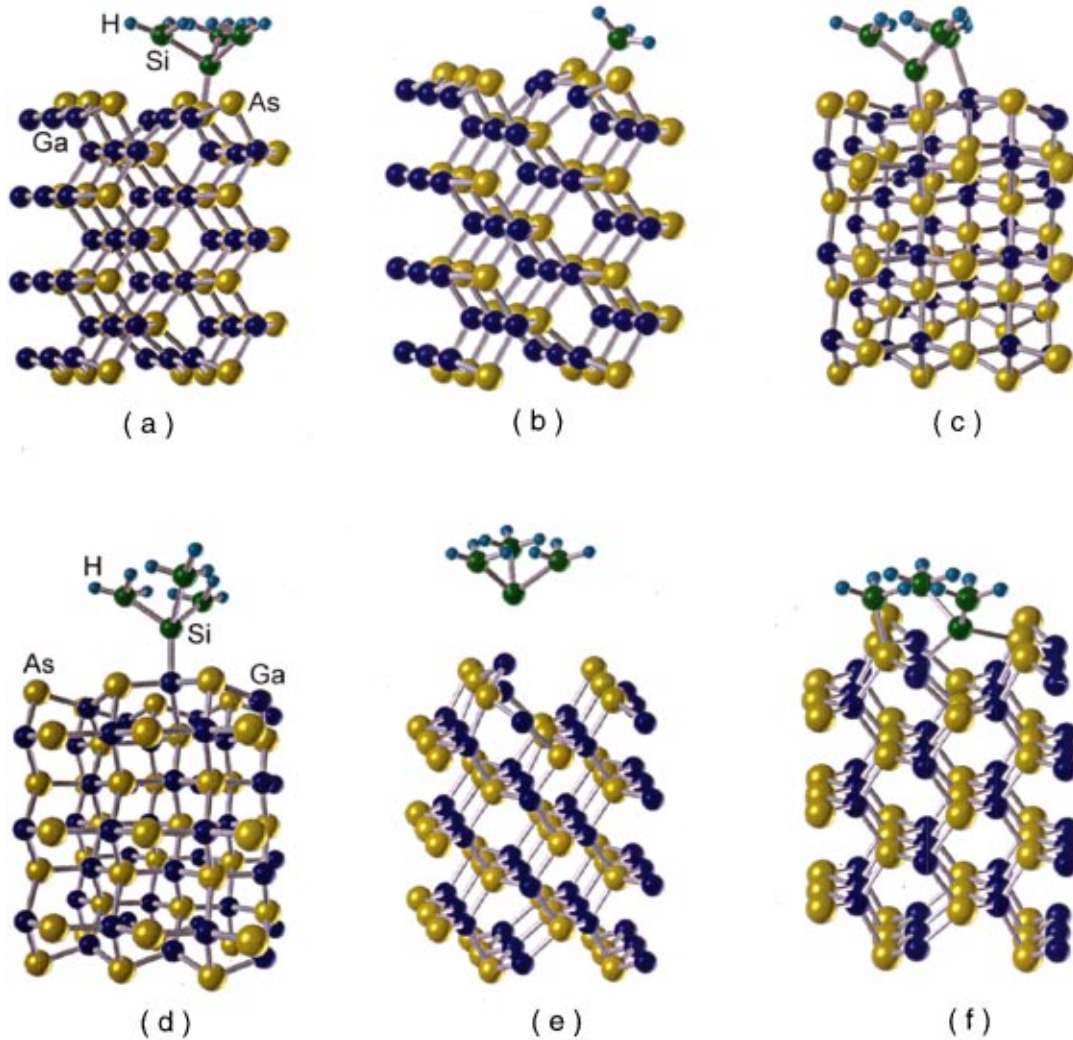


FIG. 2. (Color) Ball-and-stick model of the atomic structure of the system for certain tip positions in the displacement curves. The first row corresponds to the case where the tip (or molecule, see text) is on top of As atoms, and the second row corresponds to the case where the tip is on top of a Ga atom. (a) The atomic structure for the point *A* in Fig. 3(a), at which the As atom relaxes downwards; (b) fully relaxed structure for a free  $\text{SiH}_3$  molecule adsorbed on an As atom; (c) two-bond interaction between the tip and the surface, corresponding to point *B* in Fig. 3(a); (d) the Ga atom jumps up to form a chemical bond with the tip apex, corresponding to point *D* in Fig. 3(c); (e) the Ga atom moves together with the tip apex just before it jumps back to its original position, corresponding to point *E* in Figs. 3(c) and 3(d); (f) the tip is broken by the lateral force, corresponding to point *Q* in Figs. 3(c) and 3(d).

approximation was adopted for the exchange and correlation. Generally speaking, for the H atom a higher cutoff energy is required to achieve good convergence. However, here the role of the H atoms is merely to saturate the dangling bonds in the tip base, and for this purpose the present value of cutoff energy can be expected to be reasonable. The convergence criteria were set to  $1 \mu\text{eV}/\text{atom}$  for the total energy and  $15 \text{ meV}/\text{\AA}$  for the forces on the atoms.

The operation of the AFM in the lateral scanning mode was simulated in a stepwise, quasistatic manner by making small movements of the tip parallel to the surface along *A-A'*, *B-B'*, and *C-C'* lines (see Fig. 1) at several constant tip-surface distances. In the same way, the vertical scanning mode was simulated by moving the tip perpendicularly to the surface. We considered vertical scans over a Ga atom and over an As atom (see Fig. 1). Here, the tip-surface distance (*d*) is defined as the unrelaxed (due to the tip-surface interaction) vertical distance between the apex Si atom on the tip

and the topmost surface atom (As atoms). At each step of the scans the atoms of the first three layers of the slab and the tip apex atom were allowed to relax to their equilibrium positions for the particular tip position. Because the motion of the AFM tip is much slower than the atomic process on the surface, this kind of simulation can be expected to provide an accurate description of the imaging process.

### III. RESULTS AND DISCUSSIONS

#### A. Displacement curves

In Fig. 3, we show the energy and force curves as a function of the tip-surface distance. The comparison of the results for the scans where both the tip and the surface relax freely with those where no relaxation was allowed (all the atoms in the slab and in the tip are kept fixed at the required tip-surface distance) highlights the importance of the relaxation effects in this system. In the next two subsections, we dis-

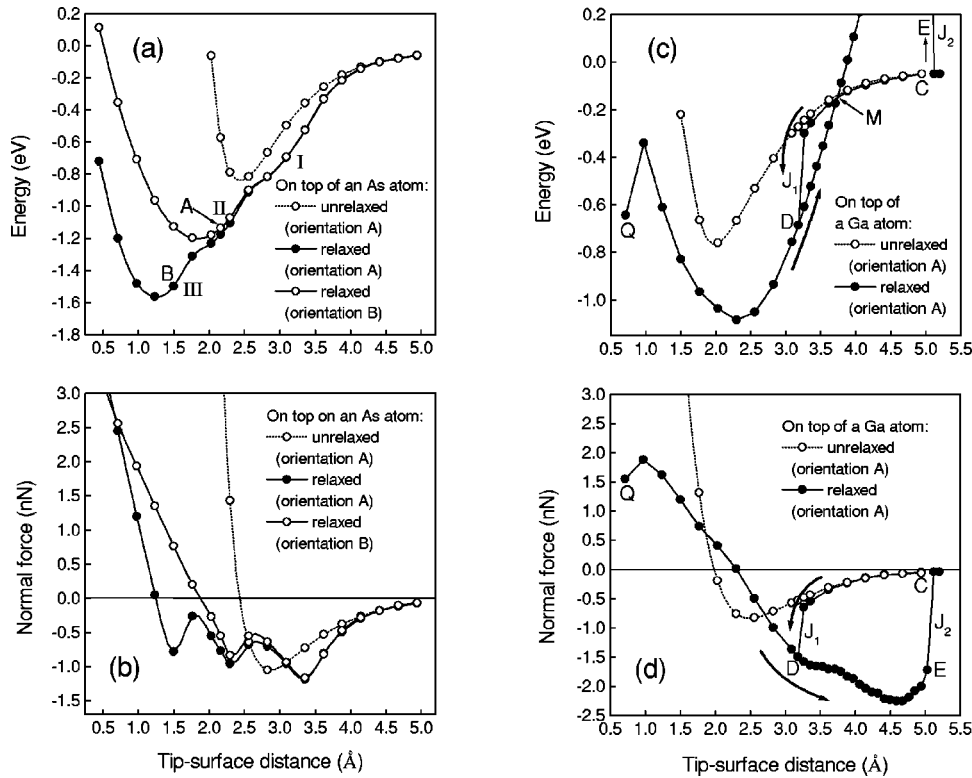


FIG. 3. The energy and force curves in the vertical scans. (a) and (b): the tip is on top of an As atom; (c) and (d): the tip is on top of a Ga atom. The atomic structures for A, B, D, E, and Q points are shown in Figs. 2(a), 2(c), 2(d), 2(e), and 2(f), respectively. The two discontinuities in the energy and the force curves are denoted by  $J_1$  and  $J_2$ .

discuss the origin of the complicated shape of those curves in the near contact region in terms of normal displacements of the tip apex and the surface atoms.

### 1. On top of an As atom

When the tip is on top of an As atom the energy curve can be divided into three parts (I, II, and III) for orientation A and two parts (I and II) for orientation B in the attractive force region [see Fig. 3(a)]. In part I ( $d > 2.5$  Å) the tip apex relaxes downwards and the As atom relaxes upwards as shown in Fig. 4(a). This lowers the energy compared to the unrelaxed condition. As the tip-surface distance is reduced to about 2.5 Å the Si apex atom and the As atom return to their original positions. In part II ( $2$  Å  $< d < 2.5$  Å), as  $d$  is further reduced, the relaxation of the Si apex atom and the As atom are reversed [see Fig. 4(a)], and the total energy decreases compared to part I. To give a clearer picture we show in Fig. 2(a) the atomic structure for point A of Fig. 3(a). This behavior is somewhat surprising at the first glance because the upward displacement of the tip apex and the downward displacement of the As atom means a repulsive force, and hence the energy in part II should be higher than in part I. However, this behavior can be understood by considering the surface relaxation effect. Once the dangling bond of the surface As atom is saturated by the tip apex Si atom, the As atom tends to return (moves downwards) to its original bulk position. In order to confirm this point, we have further calculated the absorption of a free  $\text{SiH}_3$  molecule on the As atom. The result is given in Fig. 2(b), which shows the same downward movement of the As atom after its dangling bond being saturated.

Further approach of the surface by the tip in orientation A is characterized by part III of Fig. 3(a) where the energy shows a further decrease. To show the characteristics of this

part we give the atomic structure corresponding to point B of Fig. 3(a) in Fig. 2(c). It is clear that the lower energy in this part is due to an additional bond interaction (between atoms 2 and 3 in Fig. 1). The present result indicates that even for an ideal (very sharp) AFM tip there can be more than one bond interaction between the tip and the surface in the near contact region, and this multibond interaction is not only related to the tip shape but also related to the tip orientation. In Fig. 3(b), we can see that the tip-surface interactions mentioned above induce a complicated force behavior in the near contact region.

### 2. On top of a Ga atom

When the tip is on top of a Ga atom the energy and force curves shown in Figs. 3(c) and 3(d) are characterized by two discontinuities, the jumps  $J_1$  and  $J_2$ .  $J_1$  occurs at  $d \sim 3.3$  Å as the tip approaches the surface, and  $J_2$  occurs at  $d \sim 5.1$  Å as the tip moves away from the surface. From the displacement curve of the Ga atom in Fig. 4(b), we can find that the two discontinuities are due to the jumps in the movement of the Ga atom in the normal direction.

We first analyze the origin of the  $J_1$  jump. The atomic structure for the point just after  $J_1$ , namely the D point in Figs. 3(c) and 3(d), is shown in Fig. 2(d). The Ga atom is sensitive to the presence of the tip and when the tip is close enough to the surface the Ga atom will jump up to form a chemical bond with the apex Si atom [see Fig. 4(b): the change in the Ga-Si distance before and after the jump]. The normal displacement of the Ga atom induced by the tip in this case can be as large as 1.1 Å.

To provide a supplementary understanding of this jump, we have calculated the energy change as the surface Ga atom in the pure surface system is moved artificially in the normal direction by 1.1 Å. The change in the energy is about 1.2 eV.

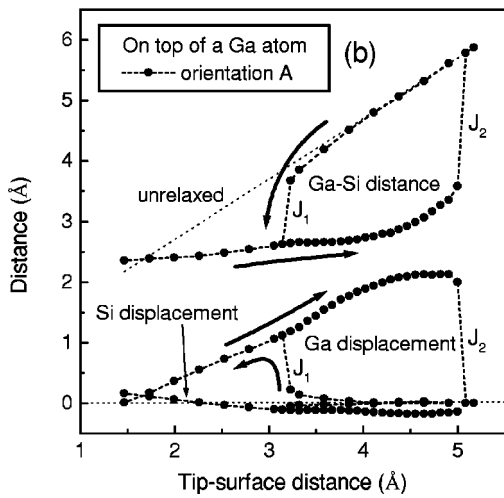
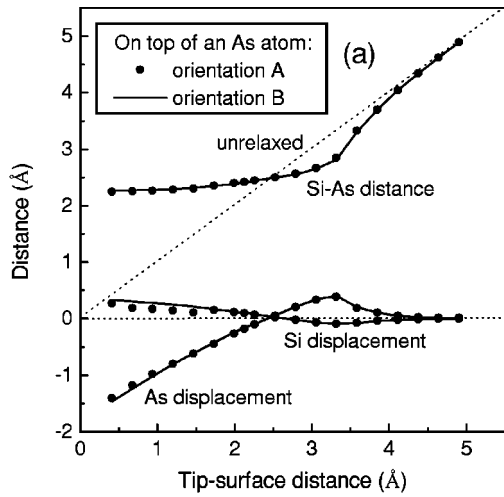


FIG. 4. Calculated normal displacements of the tip apex and the As atom (or the Ga atom) which interacts with the tip, and the distance between the tip apex and the atom interacting with it, as a function of the tip-surface distance. (a) The tip is on top of an As atom; (b) the tip is on top of a Ga atom. The two jumps of the Ga atom are denoted by  $J_1$  and  $J_2$  as in Figs. 3(c) and 3(d).

Since the typical energy of covalent bonds is about 2 eV or more, this jump is therefore understandable from the point of view of energy minimization. After the  $J_1$  jump, as the tip moves away from the surface the Ga atom will move together with the apex Si atom by up to  $\sim 1.8$  Å before it jumps back to its original position ( $J_2$  jump). This distance can be seen directly in Fig. 4(b) as the distance along the horizontal axis between the  $J_1$  and  $J_2$ . The atomic structure for the point just before  $J_2$ , namely point  $E$  in Figs. 3(c) and 3(d), is shown in Fig. 2(e). As a result of the behavior of the Ga atom, the energy and the force curves show clear hysteresis in Figs. 3(c) and 3(d).

Physically, this hysteric behavior is due to two energy minima for the Ga atom in the normal direction. For the  $D$ - $M$  part in Fig. 3(c) the energy minimum near the tip apex is deeper than the one near the surface, and for the  $M$ - $C$  part the situation is reversed. We note that the present behavior is a zero temperature result. At finite temperatures, because of

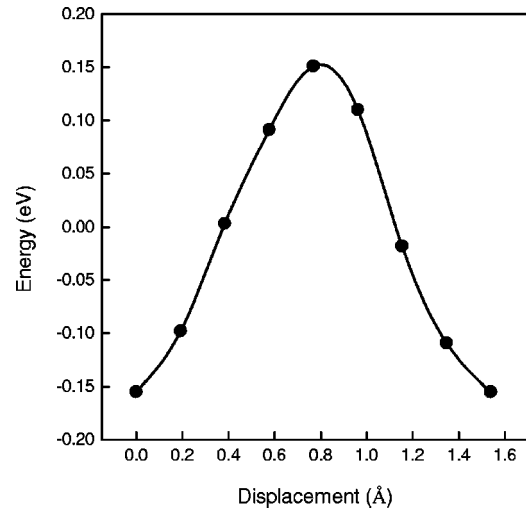


FIG. 5. Total energy variation as the Ga atom in the system corresponding to the  $M$  point in Fig. 3(c) is moved artificially from one energy minimum to another in the normal direction. The barrier between the two minima is shown to be 0.31 eV.

the reduction of the (free) energy barrier between the two minima, the hysteric behavior will weaken. The energy barrier should reach its maximum near the  $M$  point. In order to estimate the barrier at the  $M$  point, we have calculated the total energy variation as the Ga atom is moved artificially from one energy minimum to another in the normal direction. The result is shown in Fig. 5. The large barrier (0.31 eV) shown in Fig. 5 indicates that at room temperature the hysteresis should not disappear completely, and the Ga atoms could not be observed for larger tip-surface distances (see also the discussion in Sec. III B).

As the tip approaches the surface and enters the repulsive force region (contact region) we obtain an abnormal point ( $Q$ ) in the energy and force curves of Figs. 3(c) and 3(d). From the atomic structure at this point [see Fig. 2(f)] one can clearly see that, due to the large lateral force acting on the apex atom, one of the Si-Si bonds of the apex atom has been

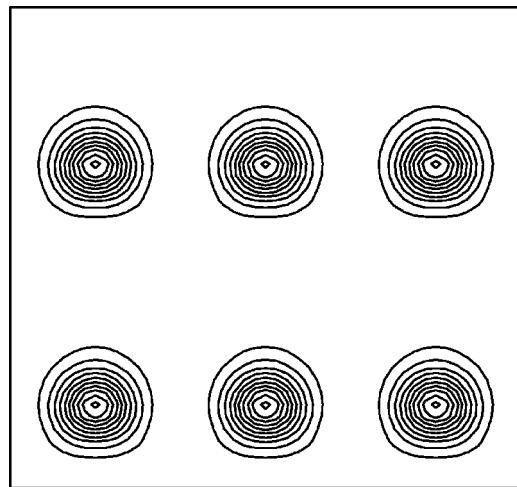


FIG. 6. Charge density in the plane 1 Å above the unperturbed surface for the electronic states with energy in the energy range (0–1) eV below the Fermi level. Note that only the sites of the As atoms are visible.

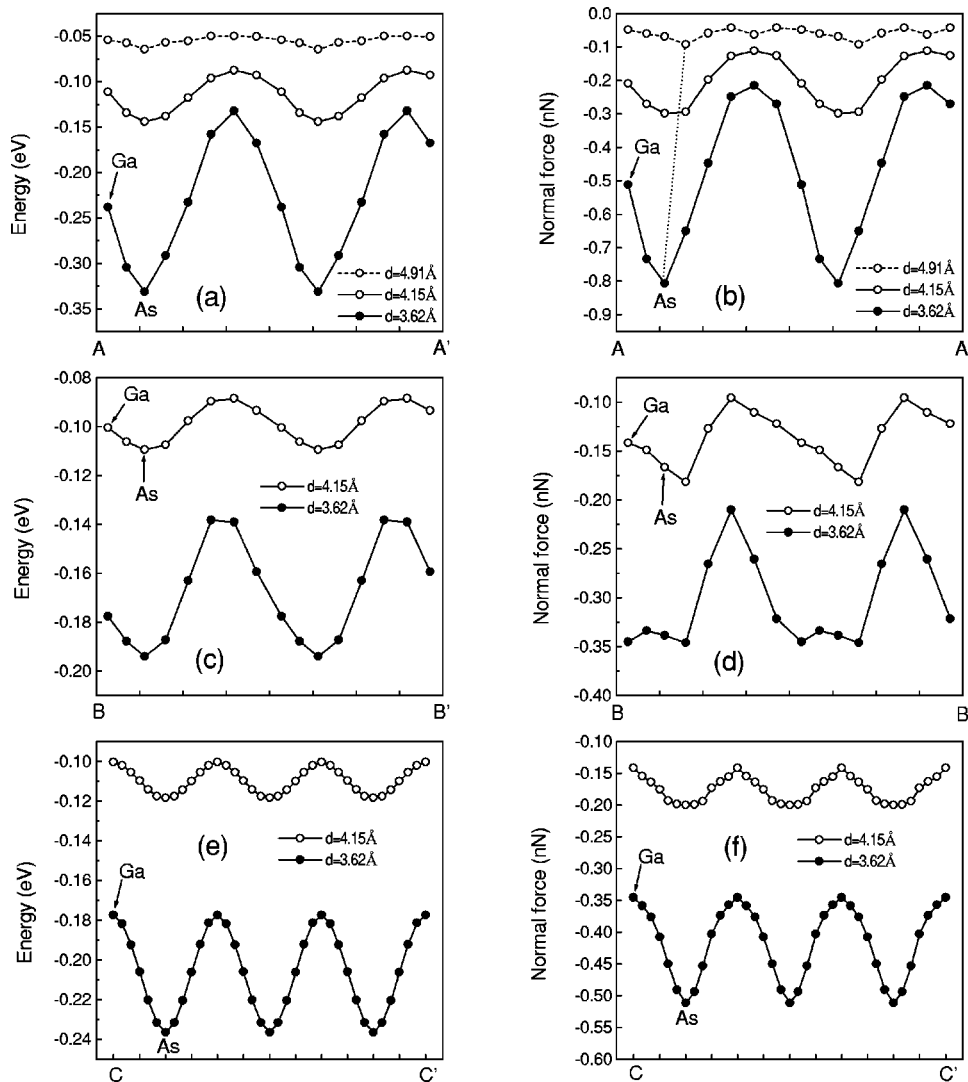


FIG. 7. Total energy and force variation as the tip (orientation  $A$ ) scans along the  $A-A'$ ,  $B-B'$ , and  $C-C'$  lines shown in Fig. 1 at different tip-surface distances: 3.62 Å (full line, white dots), 4.15 Å (full line, black dots), and 4.91 Å (dashed line, white dots). Positions of the atoms (both one on the axis of the scan and one off axis) are indicated. The dotted line in (b) shows the shift of the normal force maximum.

broken. The reason for this is the bonding between the apex atom and the surface As atoms that are nearest neighbors of the Ga atom just below the tip. It should be noted that in the present case we are using a tip containing only four Si atoms and that only the Si apex atom is allowed to relax. In a simulation with a larger tip or under real experimental conditions, these large lateral forces could be accommodated by inducing some elastic distortions in the tip structure, preventing breaking of the bond at this stage of the process. Our own experience with other tips and surfaces tends to indicate that, although some elastic distortions occur in larger tip they do not preclude breaking of the tip apex.<sup>18</sup> The importance of this result lays in the fact that large lateral (bonding) forces can develop and significantly affect the structure of the tip well before the large repulsive normal forces appear. Up to now, this was the accepted signature of the beginning of contact and possible tip and surface damage.

### 3. Relevance to recent STM observations on GaAs(110) surface

The large tip-induced normal displacements of the surface Ga atoms at small tip-surface distances provides a natural explanation to some recent near-contact STM observations on GaAs(110) surfaces.<sup>22,23</sup>

As mentioned previously, on the GaAs(110)  $1 \times 1$  relaxed surface the dangling-bond-related states of the anion are near

the Fermi level and occupied, and the ones related to the cation are empty. Under the usual STM operation conditions, where the tip-surface gap spacing is around 7 Å,<sup>22</sup> one can image either the filled dangling bonds of the surface As atoms or the empty dangling bonds of the Ga atoms by varying the sample polarity from negative to positive bias.<sup>24</sup> STM images in this conventional mode show only one of the two sublattices on the surface for each voltage polarity, and can be explained by the Tersoff-Hamann theory.<sup>25</sup> In Fig. 6, we show the charge density corresponding to the electronic states in the energy range (0–1) eV below the Fermi level in the plane 1 Å above the surface. It can be seen that only the As atoms are visible, just as experimentally observed.

Recently, Heinrich *et al.* reported a STM study of GaAs(110) surface adopting a new imaging mode.<sup>22</sup> In this new mode, a low-sample voltage (–0.75 eV) was used, and, in order to keep the current as large as that in the conventional STM mode, the width of the tunneling gap has to be decreased drastically to 2–3 Å. At this small gap spacing they found that both the As and Ga atoms become visible in the image at one sample voltage. It has to be noticed that the measured vertical tip positions at the Ga and As derived maxima in this near contact imaging mode are approximately equal, differing by only about 0.1 Å on average, and that the observed effects were reversible and not artifacts related to

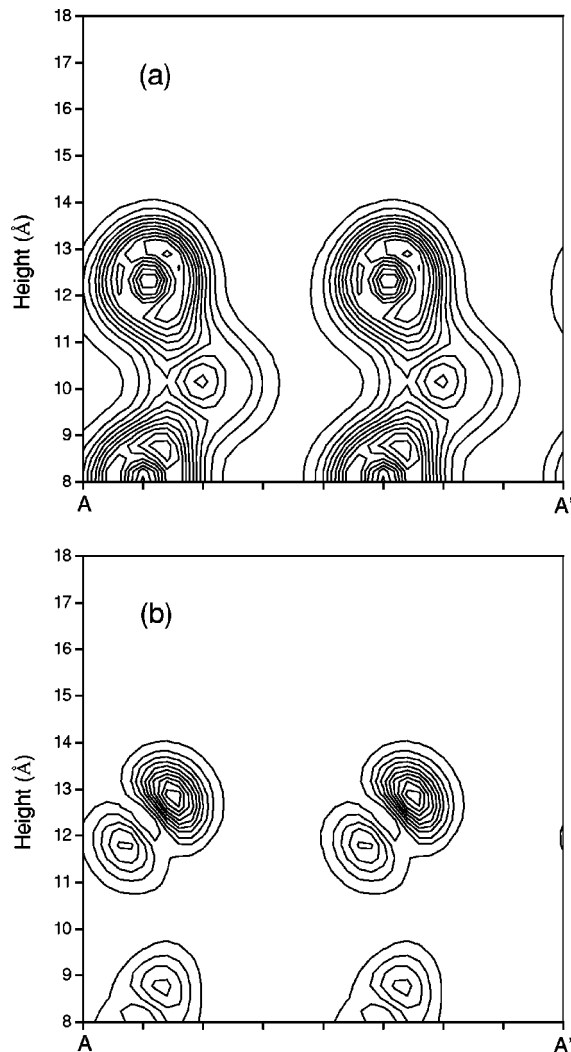


FIG. 8. The charge density in the plane through the  $A-A'$  line (see Fig. 1) and perpendicular to the surface of the unperturbed surface system: (a) total; (b) for states with the energy in the window (0–1) eV below the Fermi level. Notice the orientation of the dangling bond on surface As atoms shown in (b).

spontaneous changes of the tip structure.

It is obvious that this behavior cannot be understood just by considering the charge density of the electronic states of the unperturbed surface. At these near-contact distances the tip apex is really probing the short-range chemical interactions with the surface atoms and as a result important relaxation effects both in the tip and surface take place. These tip-induced relaxation effects change significantly the electronic properties of the surface—in particular, the nature and localization of the states around the semiconductor gap—and provide a reasonable explanation to the experimental images. In fact, the authors in Ref. 22 already suggested that, provided that the tip formed site-dependent chemical bonds with the surface atoms, these localized states will dominate the tunneling current. The present results, showing the tip-induced jump of the surface Ga atom to bond to the apex atom, provide a direct evidence for such a process. Note that the tip-surface distance required for the Ga jump obtained in our calculation (3.3 Å) is consistent with that in the STM

measurement using the new mode, and that the almost equal heights of the surface atoms in our simulations are in good agreement with the experimental result.

### B. Lateral scans

In Fig. 7, we show the calculated energy and force variations in the lateral scans along the  $A-A'$ ,  $B-B'$ , and  $C-C'$  lines. As is well known, the tip-surface force in AFM includes a short range force of chemical bond origin and a long range Van der Waals (vdW) force if other additional forces such as electrostatic forces and magnetic forces are absent. As demonstrated by Pérez *et al.*,<sup>9,10</sup> it is the chemical-bond-like force that provides the true atomic resolution. As mentioned in the Introduction, in the frequency shift AFM under typical experimental conditions<sup>12,13</sup> the quantity detected is approximately the geometric mean of the potential energy and the force.<sup>11</sup> Because in lateral scans the variations of the force and the energy generally have the same trend (see Fig. 7), the energy or the force distribution in the lateral scans obtained from the theoretical calculation can therefore qualitatively reflect the real AFM image.

Along  $A-A'$  line we have performed lateral scans for three tip-surface distances, shown in Figs. 7(a) and 7(b). It can be seen clearly that the tip-surface interaction becomes stronger as the tip-surface distance is reduced. For the tip-surface distance of 4.91 Å the variation range of the energy and the normal force are only 0.016 eV and 0.06 nN, respectively. Hence, for tip-surface distances larger than  $\sim 5$  Å it will be difficult to obtain experimentally a clear signal. As the tip-surface distance is reduced from 4.91 to 3.62 Å, the signals from both energy and normal force is enhanced by a factor of about 100. This behavior originates from the short-range chemical bond interaction. Note that in Fig. 7(b) the normal force maxima shift slightly in the direction of  $A \rightarrow A'$  along with increase of the tip-surface distance (see the dotted line in the figure). This is a clear signal of the orientation of the As dangling bond. To show the picture more clearly we give in Fig. 8 the charge density in the plane through the  $A-A'$  line and perpendicular to the surface. Figure 8(a) shows the total charge density distribution. Since the energy of dangling bonds is generally close to the Fermi level, we show in Fig. 8(b) the charge density in the energy range (0–1) eV below the Fermi energy, where the orientation of the dangling bond can be clearly visible.

When the tip scans along the  $B-B'$  line, only the As atoms can be detected in the energy distribution [see Fig. 7(c)]. In the force distribution the situation is the same for the tip-surface distance around 4.15 Å. However, when the tip-surface distance is reduced to around 3.62 Å, in addition to the As atoms, the Ga atoms can be barely distinguished. On the other hand, when the tip scans along the  $C-C'$  line, sites having the strongest signal are those of As atoms and the sites having the weakest signal are those of Ga atoms both in the energy and force curve. Hence, we conclude that, overall the Ga atoms will be “hidden” by the As atoms and only the As atoms will be visible in the image if the jump of Ga atoms does not occur (namely the surface topography is kept unchanged). This finding is consistent with the experiment.<sup>16</sup> A similar result was also obtained in the *ab initio* calculation for InP(110)-Si-tip system,<sup>18</sup> which showed that only the P sublattice is visible.

We point out that the present result indicating that only As atoms would be visible in the image, was obtained with a charge neutral Si tip. In this case the different charge states of the Ga and As atoms are not strongly reflected in the energy and the force distributions of the lateral scans. It seems possible that, if we use a negatively charged Si tip, the signal for the Ga atoms is enhanced and that for the As atoms is weakened due to the additional strong Coulomb interaction. Under this condition both Ga and As atoms on the surface may appear in the image. In fact, the very recent noncontact AFM study on InAs(110) surface<sup>17</sup> showed that, under certain experimental conditions, both As and In sites are visible in the image. This was attributed<sup>17</sup> to the additional electrostatic interaction between the tip and the surface. This suggests that further theoretical and experimental work is required to fully understand the consequences of using charged or highly polarized tips.

#### IV. SUMMARY

Using *ab initio* pseudopotential total energy techniques we have investigated the tip-surface interaction in AFM for a Si tip scanning vertically and laterally the GaAs(110) surface. From the present calculations, we can reach the following conclusions: (1) The present calculation provides evidence that the effect of surface relaxation induced by the AFM tip can be significant for some surfaces. As a result, the tip-surface force behavior in the near contact region can be complicated and strongly affected by the tip structure. The

present result of the tip-induced Ga atom jump also provides a natural explanation to some recent STM observation on GaAs(110) surface. This jump is absent on the related InP(110) surface,<sup>18</sup> which appears to be more rigid to the silicon tip. This difference causes marked differences in the displacements curves in the near contact region. We believe that the similarity between the experimental images of the two surfaces is caused by the fact that they have been collected at distances further away from the surface. (2) The present calculation shows that even for a very sharp tip there can be more than one bond interaction between the tip and the surface in the near contact region. (3) In spite of the complexities the image with real atomic resolution can be obtained by noncontact AFM if the nearest tip-surface distance can be controlled to be within 3.5–5.0 Å. (4) It seems that only the anion sublattice on the III-V(110) surfaces<sup>18</sup> can be imaged by the non-contact AFM with a charge neutral Si tip in the case that the surface topography is kept unchanged. (5) In the contact region we find situations with large lateral forces on the tip apex which may change the tip structure.

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