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Effect of tip morphology on AFM images

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Abstract. The effect of tip morphology on the atomic force microscope (AFM) image contrast for a GaAs(110) surface is investigated theoretically by considering three different tip apexes of a Si tip: (1) Si apex with a half-filled dangling bond; (2) Ga apex with an empty dangling bond; and (3) As apex with a fully filled dangling bond. It is shown that the dangling-bond state of the tip apex has significant effects on the image contrast: the Ga apex will image the As sublattice, and the As apex will image the Ga sublattice, and in the case of the Si apex, it is possible to image only the As sublattice or both the As and Ga sublattices, depending on the tip–sample separation.

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As demonstrated by different researchers, true atomic resolution can be achieved by the atomic force microscope (AFM) in the so-called non-contact (nc) mode. However, the physical origin of the image contrasts observed has not been fully understood. It was thought that the short-range tip–sample interaction from dangling bonds plays an important role in the image formation on reactive semiconductor surfaces. Intuitively, this kind of dangling-bond interaction and therefore the resulting image contrast should be affected significantly by the tip morphology, especially the dangling-bond state of the very end of the tip. This point has been corroborated by experimental evidence, for example, on a Si(111)-7×7 surface [1–3]. Very recently, Schwarz et al. [4, 5] also reported a new set of different nc-AFM images on an InAs(110) surface. The difference in the image contrast was attributed to the change in the dangling-bond state of the tip apex. However, up to now, there is no quantitative investigation of this problem, although a model analysis [6] is available for an insulator system, where electrostatic force or Van der Waals force rather than the chemical-bond interaction is dominating. In this paper, we report a theoretical investigation on the effect of tip morphology (different dangling-bond states of the tip apex) on AFM images by performing first-principles simulation for a GaAs(110) surface with a Si tip.

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1 Computation

We have considered a supercell which contains a GaAs(110) slab and a Si tip. The slab has a 2×3 in-plane size and consists of seven layers in the normal direction. The Si tip consists of four tip atoms with the three base Si atoms saturated by nine H atoms (see Fig. 1a). In order to investigate the effect of tip morphology, we have considered three different tip apexes: (1) Si apex with a half-filled dangling bond; (2) Ga apex with an empty dangling bond; and (3) As apex with a fully filled dangling bond. Hereafter, the three different tips are denoted by Si/Si, Ga/Si, and As/Si tips, respectively. The calculation is performed by using the ab initio plane-wave pseudopotential method with 9 Ry for the cutoff energy and the Γ-point for k-sampling. Optimized Troullier–Martins-type pseudopotentials are used for the atomic cores and the generalized gradient approximation (GGA) is adopted for the exchange and correlation. The operation of the AFM in the lateral scanning mode was simulated in a stepwise, quasi-static manner by making small movements of the tip parallel to the surface along A–A′, B–B′, C–C′, and D–D′ lines (see Fig. 1b) at several constant tip–surface distances (d), which distance is defined as the unrelaxed vertical distance between the tip apex 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 were allowed to relax to their equilibrium positions for the particular tip position.

2 Results and discussion

As demonstrated in [7], in the nc-AFM under typical experimental conditions the quantity detected is approximately the geometric mean of the tip–sample potential energy and the normal force. Hence, in what follows (see Figs. 2–4) we show the calculated potential energy and normal-force variations in the lateral scans along the different lines.

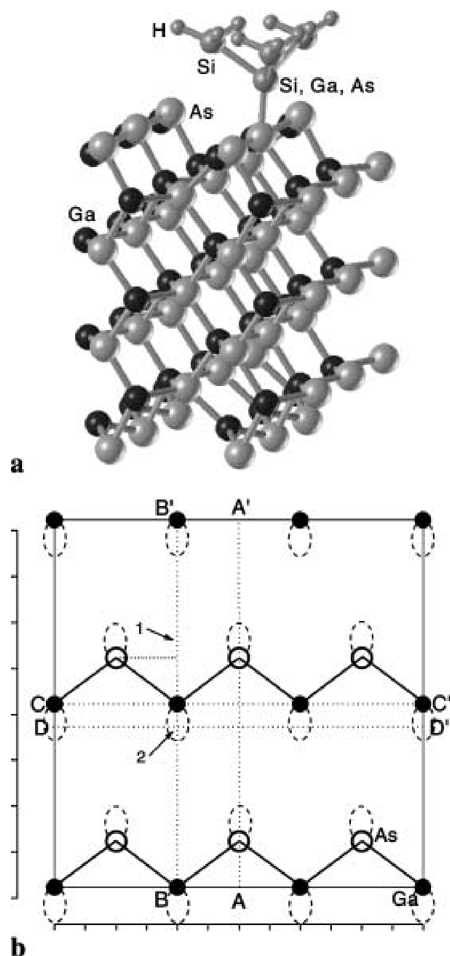

Fig. 1a,b. Side view (**a**) and top view (**b**) of the supercell. In **b** the paths along which the tip performs lateral scans are denoted by the *dotted lines*, and the dangling bonds on the Ga and As atoms are denoted schematically by *ellipses of thin dotted lines*. The distance scales for the horizontal and vertical directions in **b** are the same as those adopted in Figs. 2−4

Here, the tip–sample potential energy is determined by $E = E_{\text{tot}}(\text{tip+slab}) - E_{\text{tot}}(\text{tip}) - E_{\text{tot}}(\text{slab})$. The results indicate that, except for some special cases such as those in Figs. 2a and b where a substantial tip-induced relaxation of the surface occurs, the variation of the normal force and potential energy follow the same trend. This general feature is very useful because we can 'see' directly the qualitative image contrast from the result of the lateral scan, and we do not even need to calculate the quantity $\sqrt{|EF|}$. In this way, we can obtain the essential information which can be compared with the experimental image contrast, by performing only lateral scans along only some important paths. The much heavier computational effort for a three-dimensional scan is therefore saved.

2.1 Si/Si *tip*

Firstly, let us discuss the results for the Si/Si tip which was studied in detail in our previous paper [8], in which we showed that the scans along the A−A′ and C−C′ lines will image only As atoms. However, when the tip scans along the B−B′ line, the situation becomes relatively complicated: for the relatively small tip–surface distance $d = 3.62$ Å the surface Ga atoms, in addition to the As atoms, become barely distinguishable. In order to clarify the situation, here we performed a simulation for a smaller tip–surface distance $d = 3.38$ Å. The result is shown in Figs. 2a and 2b together with the previous results. It can be seen that as the tip–surface distance is further reduced to 3.38 Å the force signals from the Ga atoms become stronger than those from the As atoms, and the variations of the potential energy and the normal force become different. In this case there are two maxima in the force curve: one is near the As site (the site 1 in Fig. 1b), and the other is near the Ga site (the site 2 in Fig. 1b). The small shifts from the exact atomic locations are consistent with the orientations of the dangling bonds. Closer inspection of the tip–surface interaction reveals that this behavior is due to the tip-induced relaxation of the surface Ga atom. The strong force signal from site 2 in Fig. 1b indicates that the signals from the surface Ga atoms will be on the D−D′ line rather than the C−C′ line. As a result, along the D−D′ line we may see the signals from both the As and the Ga sublattices, and the situation differs from that of the C−C′ line along which only signals from the As atoms are observed. To check this point we have performed a lateral scan along the D−D′ line. The results are shown in Fig. 2c and d. We can see that the signal from Ga atoms grows with decreasing the tip–surface distance and finally a two-maximum structure is formed in both energy and force curves.

2.2 Ga/Si *tip*

The results for a Ga/Si tip are shown in Fig. 3. Along the A−A′ and C−C′ lines the results are very similar to those for the Si/Si tip. However, along the B−B′ line the behavior is remarkably different from that of the Si/Si tip: here the double-maximum structure in the force curve is absent and the maxima of the forces (for $d = 4.15$ and 3.62 Å) are slightly smaller than those from the Si/Si tip. This is because the Ga–Ga interaction between the tip and the surface is much weaker than the Ga–Si interaction for the Si/Si tip. As a result, only the As atoms on the surface will be imaged at all tip–surface distances. Along the B−B′ line there is also a small shift between the location of the energy and force maxima and the off-line position of the As atom, which reflects the orientation of the dangling bonds on the As atoms.

2.3 As/Si *tip*

For the As/Si tip, the situation is not so self-evident as in the case of the Ga/Si tip. Firstly, the interaction between the tip apex and the surface As atoms can be expected to be rather weak because of the characteristics of the As dangling bond. Secondly, although the Ga–As interaction between the tip and the surface can be strong, the surface Ga atoms are located 0.7 Å below the As atoms and the Ga–As interaction will also be weak. The final image contrast depends on the competition between the two kinds of weak interactions. In Fig. 4 it turns out that along the A−A′ line we can actually see the signals from the Ga sublattice in the energy and force curves with location shifts associated with the orientation of the dangling bond on the Ga atoms. The reason is that when the tip is over the As atoms there is almost no interaction exhibited in the energy and force curves. The scans along the

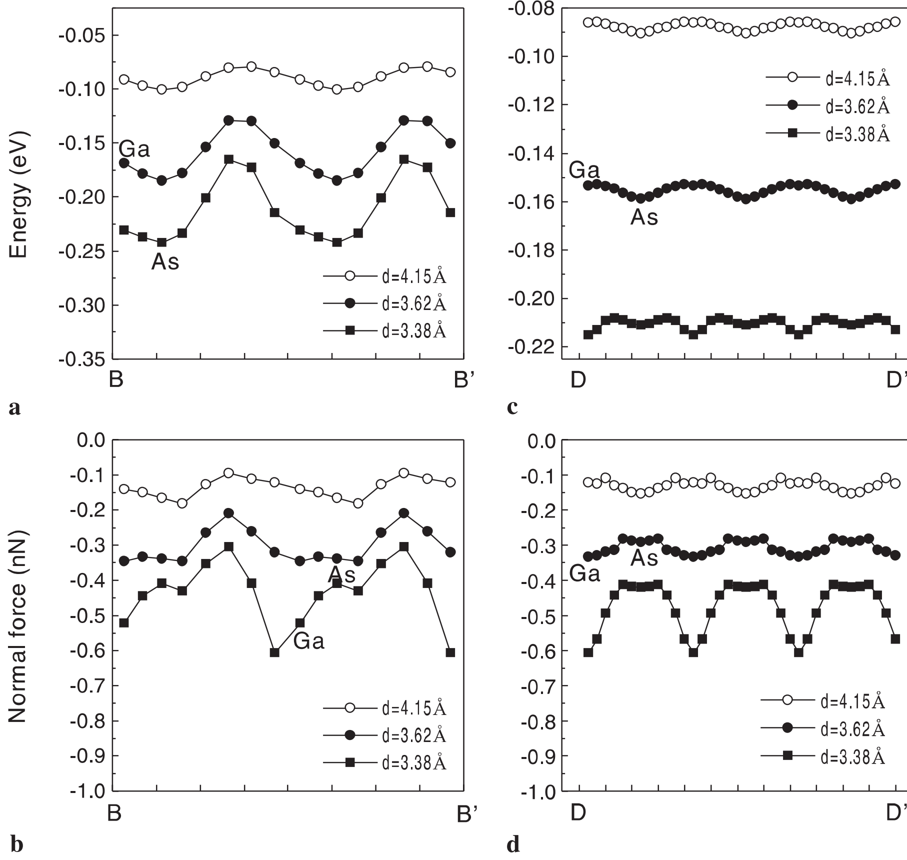

Fig. 2. Results of the lateral scans for the Si/Si tip: potential energy and normal force variations as the tip scans along the B–B′ and D–D′ lines shown in Fig. 1b at different tip–surface distances. Positions of the atoms (one on the axis of the scan and one off-axis) are indicated. The distance scale is the same as shown in Fig. 1b

Fig. 3. Results of the lateral scans for the Ga/Si tip. The notations are similar to those in Fig. 2

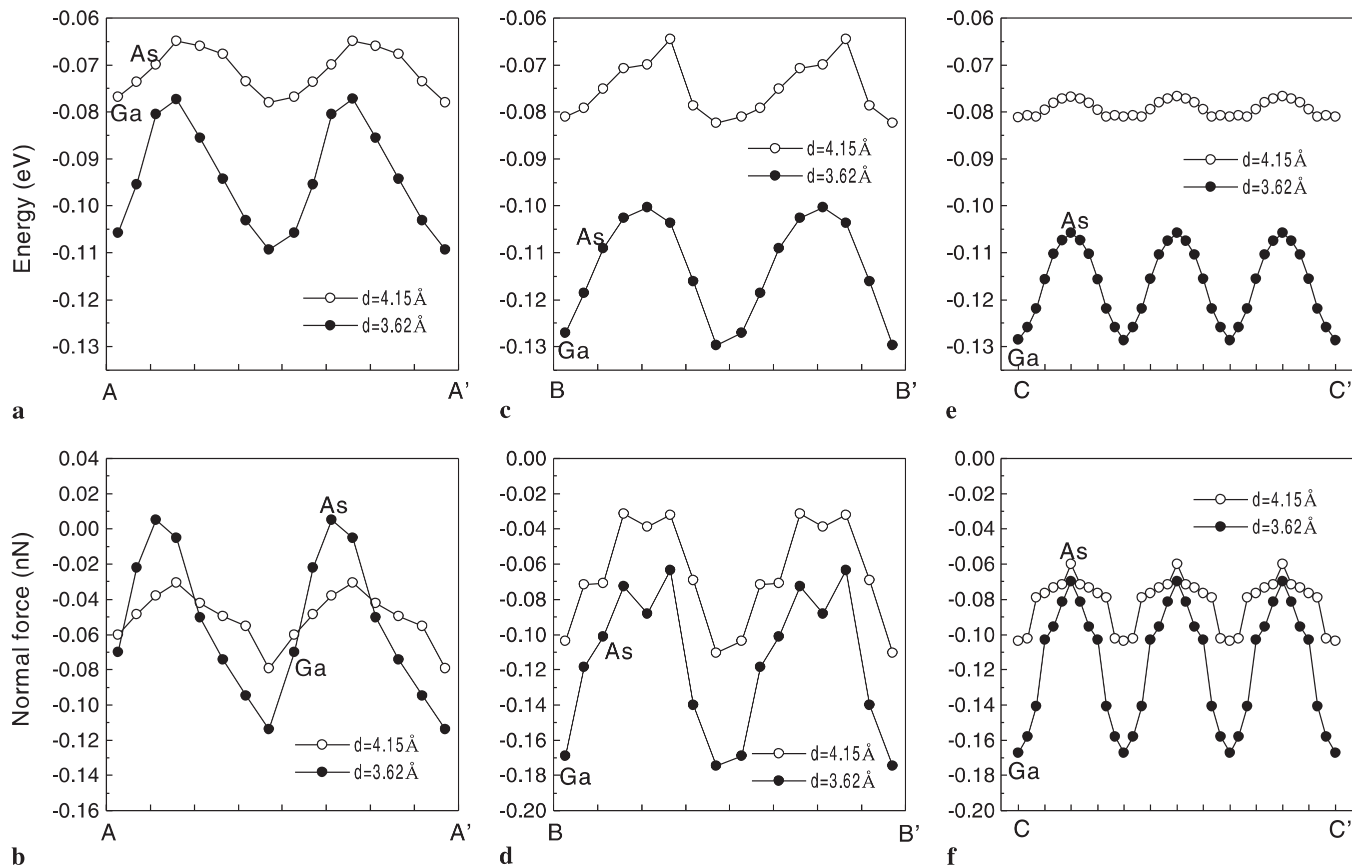

Fig. 4. Results of the lateral scans for the As/Si tip. The notations are similar to those in Fig. 2

B−B′ and C−C′ lines show qualitatively the same result: only the Ga sublattice on the surface will be imaged. This result is, in a sense, somewhat surprising because here the tip will image the lower surface atoms rather than the upper surface atoms.

3 Summary

From the above results we can reach the following conclusions: (1) for the Si/Si tip and relatively large tip–sample separation, only the As atoms will be visible in the image, which is consistent with experiment [9]. However, our calculation shows that as the tip–surface distance is reduced, it is possible to image both As and Ga sublattices, and the pattern of the image contrast will appear as a structure of bright spots with small shoulders. Our result may have some correspondences to a recent experimental report [4, 5] for a related system, InAs(110), which also showed that under certain experimental conditions the two sublattices on the surface can be resolved, and that in some cases the image contrast has also the structure of bright spots with small shoulders. (2) the change of tip apex atom from Ga to As will produce reversal in the image contrast. For the Ga/Si tip the As sublattice is imaged while for the As/Si tip the Ga sublattice is imaged. However, the topological pattern of the image contrasts are almost the same, the only difference being the strength of the image. (3) overall, the present investigation shows a significant effect of the tip morphology on the nc-AFM image formation. For this reason experimental images should be analyzed carefully considering the tip morphology.

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