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The GaAs{001} surface is widely used in the construction of microelectronic devices and has considerable technological relevance.[1] The GaAs{001} surface also displays an extraordinary variety of structures as a function of experimental conditions.[2] Characterization of these structures is critical to the development of atomistic models of epitaxial growth, and to identifying the origin of surface electronic states. Recently, a general picture of the atomic ordering of GaAs{001} surfaces has emerged, particularly for the (2x4) reconstructed surface.[3]

In connection with the characterization of GaAs single crystal surfaces, we have been investigating the possibility of utilizing the angular distributions of Ga⁺ ions desorbed from these surfaces to provide complementary structural information. These studies are potentially valuable since molecular dynamics simulations of ion induced desorption experiments have shown that the vast majority of detected atoms originate from the top three or four atomic layers.[4,5] Angular anisotropies are predicted to reflect the surface crystal structure, either through channeling and blocking of desorbing ions by other surface atoms or by direct collisions between atoms in the top three or four atomic layers, resulting in desorption along the direction of their common bond. In previous studies, for example, it has been possible to reconcile the chain rotation reconstruction associated with the GaAs{110} surface using this approach.[6]

In this paper, we examine the response of the MBE grown GaAs{001} (2x4) surface to 3 keV Ar⁺ ion bombardment by measuring the angular distribution of desorbed Ga⁺ ions. The major features of the angular distributions are easily understandable from simple collision models without having to employ an extensive calculational effort.

The experimental apparatus necessary to perform angle-resolved SIMS experiments on GaAs{001} surfaces is complex, and is described in detail elsewhere.[7] Briefly, the GaAs{001} (2x4) surfaces were prepared by molecular beam epitaxy in a Riber 2300 growth chamber. After synthesis, the wafers were transferred under vacuum ($< 1 \times 10^{-10}$ Torr) conditions into a surface analysis system. Secondary ion desorption was initiated by bombardment with a normal-incidence 3 keV Ar⁺ ion beam, operated in the static SIMS regime. The signal intensity of 20 eV secondary Ga⁺ ions was detected as a function of the in-plane azimuthal angle, ϕ, and the polar angle of detection, θ, defined as the angle between the entrance aperture (of the electrostatic sector/quadrupole mass spectrometer unit) and the surface normal.

A schematic of the ideal GaAs{001} (2x4) surface is presented in Fig. 1: the 2x periodicity in the <01$\bar{1}$> crystal direction is caused by As₂ dimer formation, and the 4x periodicity in the <011> crystal direction occurs because every fourth As₂ dimer is missing from the surface. The angular distribution of 20 eV Ga⁺ ions desorbed from this surface by 3 keV Ar⁺ ion bombardment is displayed in Fig. 2. The most intense peaks arise from atom-atom collisions between neighboring
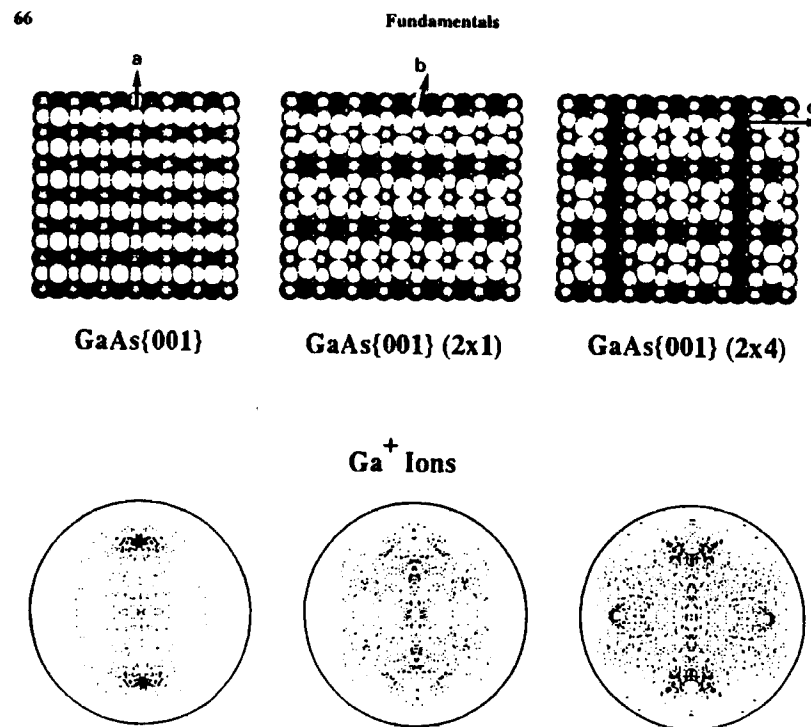
Ga⁺ Ions

Fig. 1. Top panel: Representations of three hypothetical GaAs{001} surfaces. The white balls represent surface As atoms. The slightly shaded balls represent second layer Ga atoms. Bottom panel: calculated angular distributions of 10-30 eV second layer atoms desorbed by keV Ar⁺ ion bombardment of the corresponding surface given in the top panel. The <011> azimuthal crystal direction is parallel to arrow c in the figure. The polar angle of particle emission is proportional to the distance of a spot from the center of the circle. Ion ejection mechanims a, b and c are discussed in the text.

atoms. Since the mass spectrometer is set to monitor the Ga⁺ ion signal, this type of mechanism only occurs when a third layer As atom collides with a second layer Ga atom and causes the Ga atom to eject along their mutual bond axis, as denoted by mechanism a in Fig. 1. Note that this mechanism would lead to ejection along $\phi = 90°$ and $\phi = 270°$ as observed. This direct ejection mechanism clearly dominates the distribution of ions ejected from GaAs{001} and other semiconductor surfaces, and its dominance has been attributed to be a result of the more open nature of these lattices.[5,6] By comparison, this mechanism plays only a minor part in the angular distribution of ions (or neutrals) desorbed from metal surfaces, where ejection occurs in the most open direction of the crystal surface.[8]

The second key feature in the Ga⁺ ion distributions shown in Fig. 2 is related to the shoulders associated with the major peaks at $\phi = 90°$ and $\phi = 270°$. These shoulders begin to appear at $\theta > 45°$ and persist out to the highest measurable polar
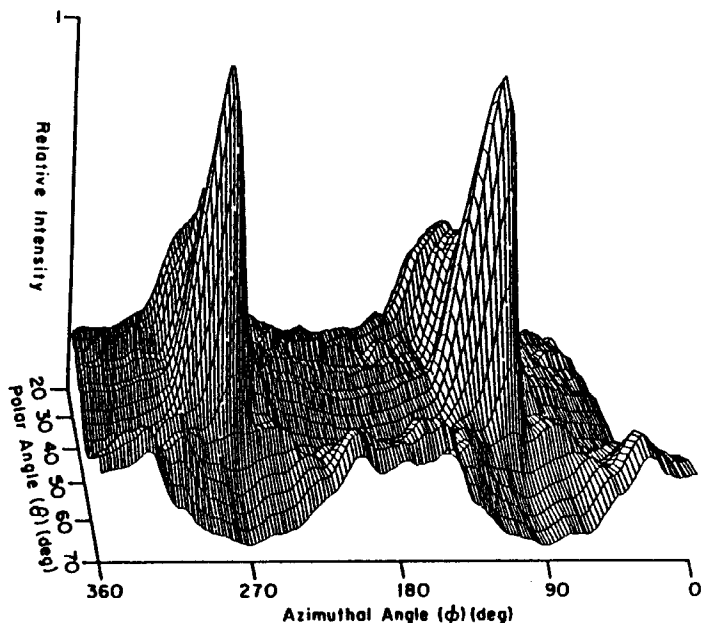
Fig. 2. The relative intensity of 20 eV Ga^+ ions desorbed by 3 keV normal incident Ar^+ ion bombardment of the GaAs{001} (2x4) surface. The polar angle is the angle of detection from the surface normal. For the in-plane azimuthal angle, $\phi=0°$ corresponds to the <011> crystal direction.

angle. This mechanism is interesting because it appears at high polar angles in an azimuthal direction that is not associated with specific atom-atom collisions. As a result of the random portion of the collision cascade, a fraction of the Ga^+ ions will take off in all directions. Some of these will be blocked by surface As_2 dimers, or may be directed between the dimers, as seen in mechanism b of Fig. 1. Many others will escape through the channel created by the missing dimers. The last important feature in the distribution are peaks seen, in Fig. 2, near $\phi = 180°$ and at $\theta > 55°$. These peaks cannot arise from any known atom-atom collision and are therefore explainable from surface channeling and blocking of Ga^+ ions ejected due to the random part of the collision cascade, shown by mechanism c in Fig. 1. The Ga^+ ions cannot eject at small values of θ since they are blocked by overlaying As atoms. At large values of θ, however, they can escape through the channel created by the missing As_2 dimers. The minimum at $\phi = 180°$ is due to blocking by an As_2 dimer across the row.

To confirm the simple arguments presented above, and to provide a sound theoretical basis for more quantitative studies, it is really necessary to perform computer simulations of the ion-impact event. Recently we have shown that calculations performed for Si crystals, where the interaction potentials are known, well predict the measured angular distributions from GaAs surfaces.[5] This agreement is possible since the bulk crystal structures of Si and GaAs are closely related and because the response of a solid to keV ion bombardment is influenced more strongly by structure than by chemical bonding forces.

Results of these calculations for the {001}, {001}(2x1) and {001}(2x4) surfaces are shown in the bottom part of Fig. 1. All of the computational details associated with these simulations have been discussed previously.[5] These distributions are for the second layer Si atoms which are found to eject as they are crystallographically equivalent to the Ga atoms shown by the grey spheres of Fig. 1. For the unreconstructed {001} surface, the Ga distribution would be expected to exhibit only two peaks at $\phi = 90°$ and $\phi = 270°$, with no structure found at higher polar angles and no intensity at $\phi = 0°$ and 180° or $\theta < 45°$. These additional features must arise entirely from the reconstruction process. Note also that the (2x1) reconstruction does not yield any intensity along $\phi = 0°$ and 180°. As discussed above, this intensity is possible only because of the channel created by the missing row of As_2 dimers found in the (2x4) surface. A detailed analysis of the atomic trajectories leading to these distributions[9] is fully consistent with the simpler, intuitive arguments developed in the previous section.

We have presented the angular distributions of Ga^+ ions desorbed from a MBE grown GaAs{001}(2x4) - As terminated surface. We show conclusively that the angular distributions are dominated by the surface structure. Analysis of the secondary ion angular distribution in conjunction with molecular dynamics simulations confirms that there are open channels parallel to the <011> direction of the GaAs{001} (2x4) surface, in accord with previous theoretical and STM studies. This technique therefore represents a new approach to examining, in detail, the structure of surfaces.

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