

Atomic geometry and dynamics of the GaSb(110) surface

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The structure of the relaxed GaSb(110) surface has been determined by mass-resolved Rutherford backscattering of He⁺ ions. From measurements of ion blocking angles it is concluded that the relaxation involves a rotation of the Ga-Sb surface bond by an angle of $\omega = 29^\circ \pm 7^\circ$ out of the surface plane. The bond lengths at the surface are shown to remain unchanged. The root-mean-square thermal vibration amplitude of the surface atoms is found to be enhanced with respect to the bulk amplitude by a factor of 1.5 ± 0.2 .

The atomic structure of the relaxed (110) surface of III-V compound semiconductors has been the subject of numerous low-energy electron-diffraction (LEED) investigations. The structure model initially proposed by Duke and his co-workers¹ is shown in Fig. 1. The relaxation is characterized by the angle ω between the plane of the uppermost chain of group III and V atoms and that of the truncated bulk surface. Until recently it was commonly accepted that ω lies in the range $25^\circ < \omega < 31^\circ$.² However, in a reevaluation of the LEED data from GaAs(110) by Duke, Richardson, and Paton,³ a new model with $\omega = 7^\circ$ was introduced, which was only slightly less favorable than the relaxation of $\omega = 29^\circ$. Also for the very similar GaSb(110) surface these two models seem nearly indistinguishable to within the accuracy of the x-ray *R*-factor analysis given in Ref. 4. The controversy is further heightened by very recent ion channeling results on GaAs(110) which disagree with the 29° model and favor the 7° model.⁵

In this Rapid Communication we report the first structure determination of a compound semiconductor surface, based on mass-resolved Rutherford backscattering. Results on the GaSb(110) surface are presented, which rule out the 7° model and fully confirm the 30° relaxation model initially proposed by Duke, Paton, and Kahn⁴ for the GaSb(110) surface. Contrary to LEED, the technique of ion channel-

ing and blocking used here is highly sensitive to displacements of atoms parallel to the surface plane. Such parallel displacements must occur if all bond lengths in the relaxed surface remain unchanged. Our results indeed show that the relaxation is purely bond-length conserving, and rule out the alternative possibility that the relaxation involves normal displacements only.⁶ Accurate values for the bond rotation angle ω and the root-mean-square (rms) surface vibration amplitudes $\langle u_s^2 \rangle^{1/2}$ have been determined by fitting the experimental results with Monte Carlo computer simulations of the experiment in which both ω and $\langle u_s^2 \rangle^{1/2}$ are free parameters of the fit. The surface vibration amplitudes are found to be strongly enhanced with respect to the bulk, for which a simple explanation is given.

Atomically clean and mirrorlike GaSb(110) surfaces were produced by cleavage in the UHV ion scattering chamber. LEED showed a sharp (1×1) pattern. Backscattered ions were simultaneously analyzed in energy and angle with a toroidal electrostatic analyzer⁷ having an energy resolution of $\Delta E/E = 4 \times 10^{-3}$ and an angular resolution better than 0.3° . Experiments were performed on three different cleaved surfaces, using about six beam spots on each surface. The accumulated beam dose on each beam spot was kept below 6×10^{14} ions/cm², to ensure that beam damage effects were negligible. The experiments were performed within 1 h after each cleavage in a pressure below 1×10^{-8} Pa.

A parallel beam of 174-keV He⁺ ions was aligned with the $[\bar{1}\bar{1}2]$ channeling direction (Fig. 1). Backscattered ions were detected in the $(\bar{1}10)$ plane for exit angles with respect to the surface plane ranging from 10° to 30° , while keeping the direction of the incident beam fixed.⁸ The energy spectrum then shows two well-resolved "surface peaks," corresponding to large-angle Rutherford backscattering from Ga or Sb atoms in the surface region. For a hypothetical static lattice with an ideal bulk-truncated surface only the topmost atoms of the $[\bar{1}\bar{1}2]$ rows would contribute to the surface peaks, since the deeper lying atoms are completely shadowed. However, thermal vibrations and static displacements resulting from surface relaxation render the shadowing of subsurface atoms less effective, resulting in nonzero hitting probabilities for these atoms and an increase of the surface peak intensities. By definition the hitting probability of the first atom in each row is equal to one. The sum of the hitting probabilities of the atoms along the row is called the number of atoms per row. The intensities of the Ga and Sb surface peaks have been converted into the number

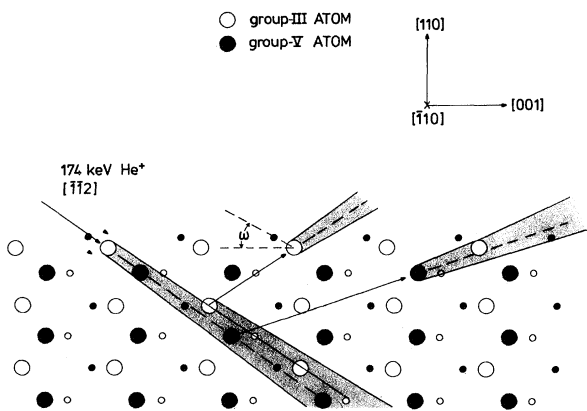


FIG. 1. View of the $(\bar{1}10)$ scattering plane perpendicular to the relaxed (110) surface of a III-V compound semiconductor. Small and large circles refer to different scattering planes. For illustration only a few of many possible shadowing and blocking cones are shown.

of atoms per $[\bar{1}\bar{1}2]$ row, visible to both beam and detector, by comparison with the backscattering intensity from a well-known standard.⁹ The accuracy of this conversion is estimated to be $\pm 5\%$.

The Ga and Sb surface peak intensities each exhibit minima for directions in which ions backscattered from subsurface Ga and Sb atoms are blocked off by an atom in or near the surface. The measured surface peak intensities for Ga and Sb versus exit angle are shown in Fig. 2. Distinct minima are observed at various surface blocking directions, from which, in principle, the atomic geometry can be derived by use of simple triangulation.¹⁰ However, the shapes of these

minima are somewhat distorted by multiple small-angle scattering effects along the outgoing path of the ions. To properly account for this, "full crystal" Monte Carlo computer simulations of the backscattering experiment have been performed for a range of different atomic geometries and enhanced surface vibration amplitudes (solid lines in Figs. 2 and 3), in search for the best fit with the data. In these simulations a Molière scattering potential has been used to calculate the small-angle deflections giving rise to shadowing and blocking. Lattice thermal vibrations were treated as isotropic Gaussian distributed displacements with one-dimensional rms amplitudes of $\langle u_x^2 \rangle^{1/2} = 0.122 \text{ \AA}$ and $\langle u_y^2 \rangle^{1/2} = 0.104 \text{ \AA}$ for bulk Ga and Sb atoms.¹¹ The surface vibrations were enhanced isotropically by a factor $S = \langle u_s^2 \rangle^{1/2} / \langle u_b^2 \rangle^{1/2}$, with S ranging from 1.0 to 1.8. The enhancement was taken equal for Ga and Sb atoms. Monte Carlo computer simulations were done for a large series of

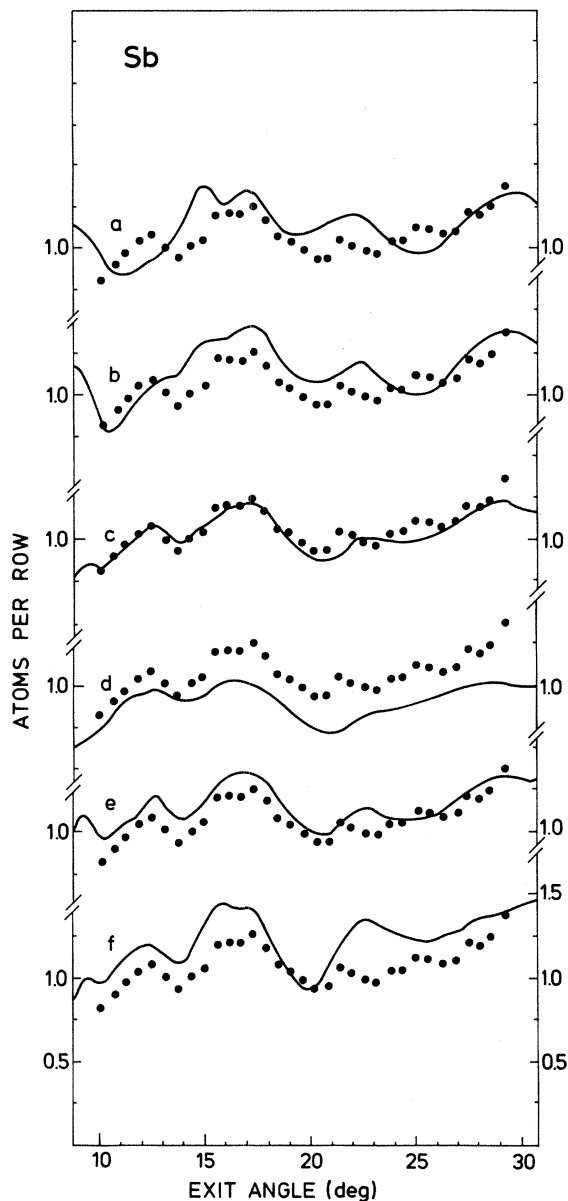


FIG. 2. Measured blocking curve for ions scattered from Sb atoms is indicated with dots. Computer simulations for several possible relaxations and enhancements of surface vibrations S are drawn with solid curves. a-e: rotational relaxation model (a: $\omega = 0^\circ$, $S = 1.5$; b: $\omega = 10^\circ$, $S = 1.5$; c: $\omega = 30^\circ$, $S = 1.5$; d: $\omega = 30^\circ$, $S = 1.0$; e: $\omega = 30^\circ$, $S = 1.8$). f: bond relaxation model ($\omega = 26.5^\circ$, $S = 1.4$).

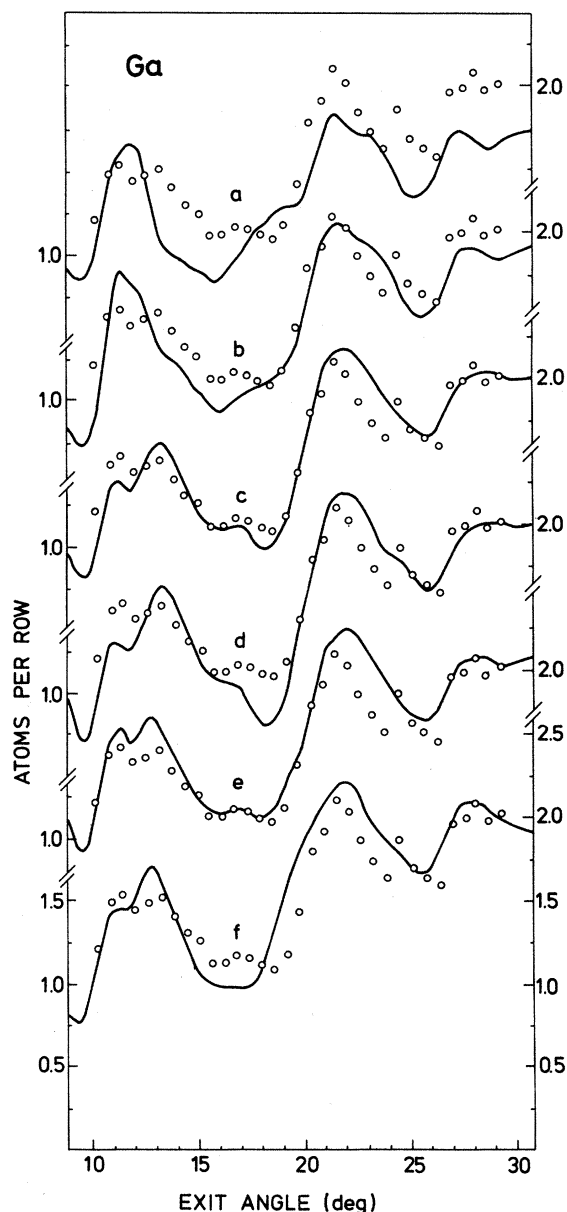


FIG. 3. As Fig. 2 but for ions scattered from Ga atoms.

bond-length-conserving rotations and enhancement factors. The coordinates of the top layer Ga and Sb atoms in the simulation model follow from the requirement that all bond lengths remain unchanged.¹² Blocking patterns simulated for $\omega = 0^\circ$ (bulk terminated), 10° , and 30° at a surface vibration enhancement of $S = 1.5$ are shown in curves a, b, and c of Figs. 2 and 3. The fit to the data is excellent for $\omega = 30^\circ$ but poor for $\omega = 0^\circ$ and 10° . Note that there are no additional adjustable parameters, i.e., experimental and simulated blocking curves are to be compared on an absolute scale. Variation of the surface vibration amplitude at $\omega = 30^\circ$ results in a best fit for $S = 1.5$. Curves d and e show simulated blocking patterns for $\omega = 30^\circ$ with $S = 1.0$ and $S = 1.8$. For the present scattering geometry, the Sb backscattering data appear to be more sensitive to variations of ω and S than the Ga data.

The quality of the fits was assessed by evaluating the goodness-of-fit criterion χ_v^2 defined by

$$\chi_v^2 = \frac{1}{\nu} \sum_{i=1}^N \frac{(Y_{i,\text{simul}} - Y_{i,\text{obs}})^2}{\sigma_i^2},$$

where N stands for the number of discrete exit angles for which the backscattering yield was measured, $Y_{i,\text{obs}}$ is the number of counts registered by the detection system in the angular channel i , and $Y_{i,\text{simul}}$ is the number of counts expected on the basis of the computer simulations. The number of degrees of freedom ν equals $N - 2$ because there are two independent parameters, ω and S , to be obtained from the fitting procedure. As the count rate is Poisson distributed the statistical standard deviation of the number of counts is taken $\sigma_i = (Y_{i,\text{obs}})^{1/2}$. Figure 4 shows the χ_v^2 values for Sb in a contour plot with ω and S as variables. A single deep minimum is found at $\omega = 29^\circ \pm 4^\circ$ and $S = 1.5 \pm 0.2$. The quoted error margins follow from the criterion that a change in χ_v^2 by more than $\Delta\chi_v^2 = 1$ is a significant deviation from the best fit.¹³ A rotation by $\omega = 7^\circ$ (Refs. 3 and 5) yields $\chi_v^2 = 7.7$ and is therefore ruled out. For Ga the best fit is independently obtained at precisely the same values, albeit with larger error margins.

Finally, we have tested the "bond relaxation" model⁶ in which a bond rotation of $\omega = 26.5^\circ$ is achieved by normal displacements only, i.e., an inward movement $\Delta z = -0.54 \text{ \AA}$ for Ga and outward movement $\Delta z = +0.22 \text{ \AA}$ for Sb. The absence of parallel displacements has been suggested by photoemission and isochromat spectroscopy data.^{14,15} The simulated ion blocking patterns for this model (curve f in Figs. 2 and 3) yield a poor fit to the Ga backscattering data and disagree strongly with the Sb data. Thus the bond relaxation model, which by LEED analysis is all but indistinguishable from the bond rotation model,³ can be ruled out on the basis of the present ion scattering results.

In conclusion, the top layer relaxation in the GaSb(110)

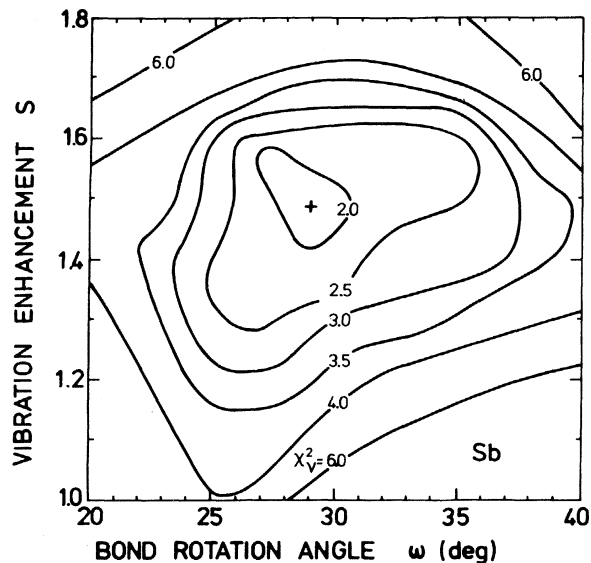


FIG. 4. Contour plot of the goodness of fit, χ_v^2 , between data for Sb and simulation vs bond rotation angle ω and enhancement of the surface vibrations.

surface is best described by the model of Fig. 1 with a bond-length-conserving rotation of $\omega = 29^\circ \pm 4^\circ$. This result is in excellent agreement with the $\omega = 30^\circ$ LEED model and rules out the $\omega = 7^\circ$ model.⁴ The anomalous enhancement of the rms surface vibration amplitude by a factor of 1.5 is intriguing. Recent total-energy calculations by Chadi¹⁶ indicate for the very similar GaAs(110) surface, that there is a nearly zero restoring force on the top layer when the Ga and As atoms in this layer are both displaced up to 0.1 \AA in either the $[\bar{1}10]$ or the $[1\bar{1}0]$ direction. For these displacements the change in total energy is 1 meV, much less than the energy involved in thermal vibrations. As a result, the vibration amplitudes are expected to be particularly large in these directions. This is likely to be true for the GaSb(110) surface too and would explain the observed anomalous enhancement.

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