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Atomic Displacements in the Si(111)-(7×7) Surface

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The parallel and perpendicular displacements of atoms in the first few layers of Si(111)-(7×7) have been determined with use of ion scattering. It was directly observed that the major reconstruction of this surface involves ~ 0.4 Å displacements perpendicular to the surface.

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The determination of the atomic positions of atoms in reconstructed semiconductor surfaces is a continuing challenge to the surface scientist. The primary structural tool, low-energy electron diffraction (LEED), can be used in a straightforward manner to determine the periodicity of the surface arrangement, but has been less successful in unambiguously establishing the actual atomic positions. In this Letter we report on an ion-scattering study of the Si(111)-(7×7) surface. The experimental results provide the first straightforward and definitive evidence that the major reconstruction in this surface involves vertical displacements of ~ 0.4 Å. We have also found that the lateral strain is small, much less, for example, than that observed in the Si(001)-(2×1) case.[1] In this paper we discuss the acquisition and analysis of these results and their implications for the various models of the Si(111)-(7×7) surface.

The ion-scattering technique for surface-structure determination makes use of the shadowing effect[2] which occurs for an ion beam incident along a major crystal axis direction. The first atom in an ideal string of atoms parallel to the incident beam forms a shadow cone which reduces the probability of close encounters between the incident ions and atoms further along in the string. In a reconstructed surface the first atom may not be aligned with the atomic row and the shadowing is reduced. The energy spectrum of the backscattered ions contains a high-energy surface peak (SP) due to interactions of the beam with the exposed surface atoms. The SP is a quantitative measure of the shadowing effect.

The apparatus for this study has been described elsewhere.[1] Briefly, it consists of a UHV system coupled to a Van de Graaff accelerator which produces He^+-ion beams collimated to ~ 1 mm^2 over the range of 0.1–4.0 MeV. The system contains visual-display LEED apparatus, Auger apparatus, sample-cleaning equipment, and a sample manipulator for channeling orientation. Also held on the manipulator is a scattering standard consisting of a heavy element implanted at low energy into Si. Scattering from this standard, calibrated against a known implanted standard,[3] can be compared to the scattering from the sample to obtain an absolute determination of the areal atomic density in the SP.

The Si surface was cleaned by Ar sputtering and annealing. The sample was considered suitable when (1) there was no indication of an oxygen Auger signal to within the noise limitations of the Auger apparatus; (2) the carbon KLL signal was $<1/1000$ of the Si LVV line; and (3) the LEED pattern was a well-developed 7×7 structure. Rutherford backscattering analysis indicated a trace of heavy-metal contaminants in the surface region of total concentration $\lesssim 2\times10^{13}$ atoms/cm^2. These impurities were not detectable by Auger analysis.

We report measurements of the ⟨111⟩ SP intensity as a function of energy (0.15 to 1.0 MeV) and the ⟨001⟩ SP intensity as a function of energy and tilt angle about the channeling direction. An accurate determination of the SP intensity is obtained by using a grazing exit-angle technique for the scattering geometry and detector placement; this provides optimum depth resolution and minimum background subtraction. The SP intensity was extracted from backscattering energy distributions of the type shown in Fig. 1 and is accurately converted to atoms/cm^2, or monolayers, through the use of the calibrated standard. The statistical error associated with the determination of the SP is less than ± 2% and relative values at different energies and temperatures are correspondingly accurate. The absolute determination of the SP may involve systematic errors associated with the standard (~ 2%) and the assumption of Rutherford scattering for Si (< 2%). We have ascribed a total error of ± 5% to the SP.

The ⟨111⟩ SP intensity as a function of incident ion energy at room temperature is shown in Fig. 2(a). The SP is measured in terms of atoms/row. One atom/row corresponds to three monolayers, since in the ⟨111⟩ direction of a Si(111) surface the atom strings begin at three different layers. The increase of the SP as a function of energy is expected, based on the general ideas of the shadowing concept. The full curve is obtained from computer simulations using a bulklike surface structure.[2] They include bulk vibration amplitudes (bulk Debye temperature of 543 °K) and two-atom correlations.[4] In general, there is rather good agreement between the measured and calculated values, particularly at low energies. The small deviations that appear at high energy can be due to either laterally displaced surface atoms or enhanced vibration amplitudes, or both. Computer simulations using reconstructed surfaces

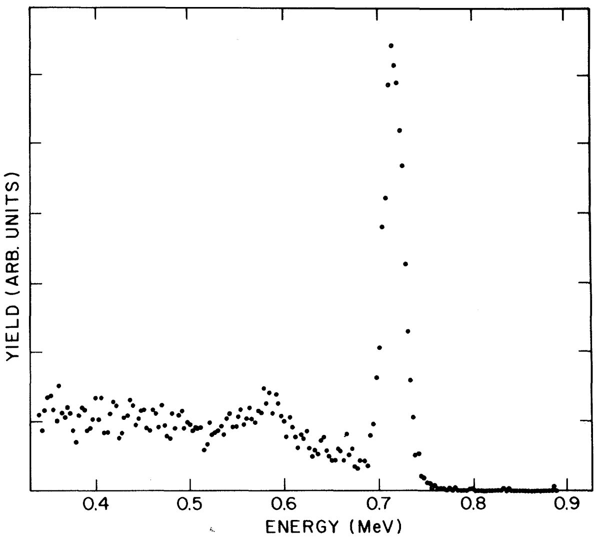

FIG. 1. Backscattered spectrum for 1-MeV He$^+$ incident to a Si(111)-(7×7) surface.

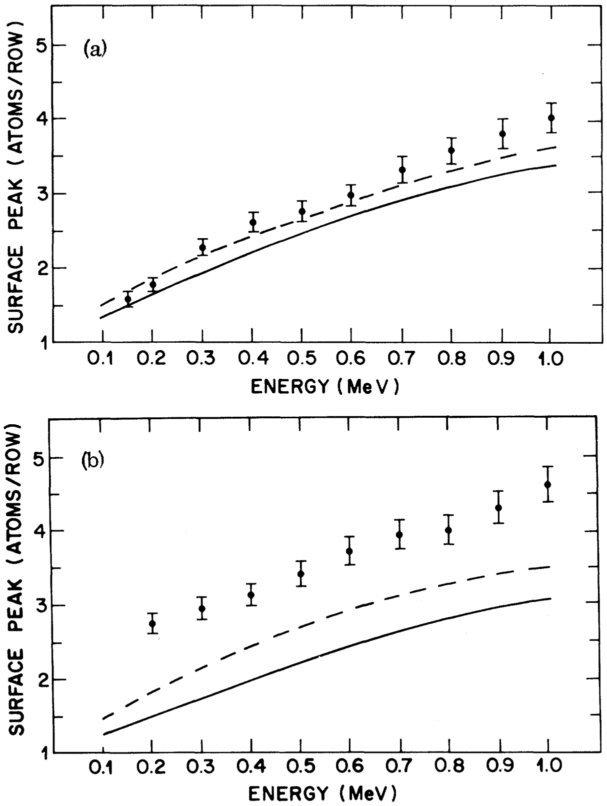

FIG. 2. Surface peak intensity as a function of incident ion energy for (a) the ⟨111⟩ direction at 300 °K and (b) the ⟨001⟩ direction at 300 °K. The full and broken curves are calculated values at 300 °K for a bulklike surface and a bulklike surface with enhanced vibration amplitudes, respectively. In the ⟨111⟩ and ⟨001⟩ directions one atom per row is equivalent to three and two monolayers, respectively.

allow us to set an upper limit of 0.15 Å transverse displacements in one to two layers.

Experiments performed in the ⟨111⟩ direction are only sensitive to atom displacements *parallel* to the surface. By orienting the beam along a nonnormal axial channeling direction, such as the ⟨001⟩, atom displacements *perpendicular* to the surface are detected. The measured SP intensity for the ⟨001⟩ direction is compared to the simulation results in Fig. 2(b). The large discrepancy between experiment and simulations for a bulklike surface (full curve) is in marked contrast to the ⟨111⟩ data [Fig. 2(a)]. Since the ⟨001⟩ direction in Si(111) consists of two monolayers—i.e., 1 atom/row corresponds to two monolayers—these data indicate that at least two monolayers have large displacements perpendicular to the surface.

By measuring the SP as a function of small variations of the incident angle further geometrical information about the displacements can be obtained.[5] Such an angular scan was made about the ⟨001⟩ direction in the {110} plane using 500-keV He$^+$. The results are shown in Fig. 3(a) along with computer simulations for all the atoms in each of the first two monolayers contracted from 0 to 0.61 Å perpendicular to the surface. The calculated curves for perpendicular displacements of 0.12 to 0.37 Å are very asymmetric, as expected for displacements of the order of the shadow-cone radius. Much larger displacements yield symmetric results; the displaced atom simply adds 1 atom/row but has no effect on the shape of the curve. If half the ⟨100⟩ strings have the first atom displaced upward and the other half have the first atom displaced downward by the same amount the angular scan would always appear symmetric [Fig. 3(b)]. The results for displacements of 0.24 Å or less still fall well below the data, but the fit for the 0.49-Å displacement is fairly good. Although from the results in Fig. 3 it is not clear if the atoms are moved inward, outward, or a combination of both, the presence of large perpendicular displacements in two layers is firmly established.

A parameter of some uncertainty in the calculation is the surface vibration amplitudes. Surface-vibration–enhancement factors can be extracted from LEED experiments; the largest value in the recent literature yields an enhancement in the mean-square amplitude of a factor of 3.8, corresponding to a surface Debye temperature of 330 °K.[6] As an extreme case we have calculated the ⟨100⟩ surface peak using an isotropic enhance-

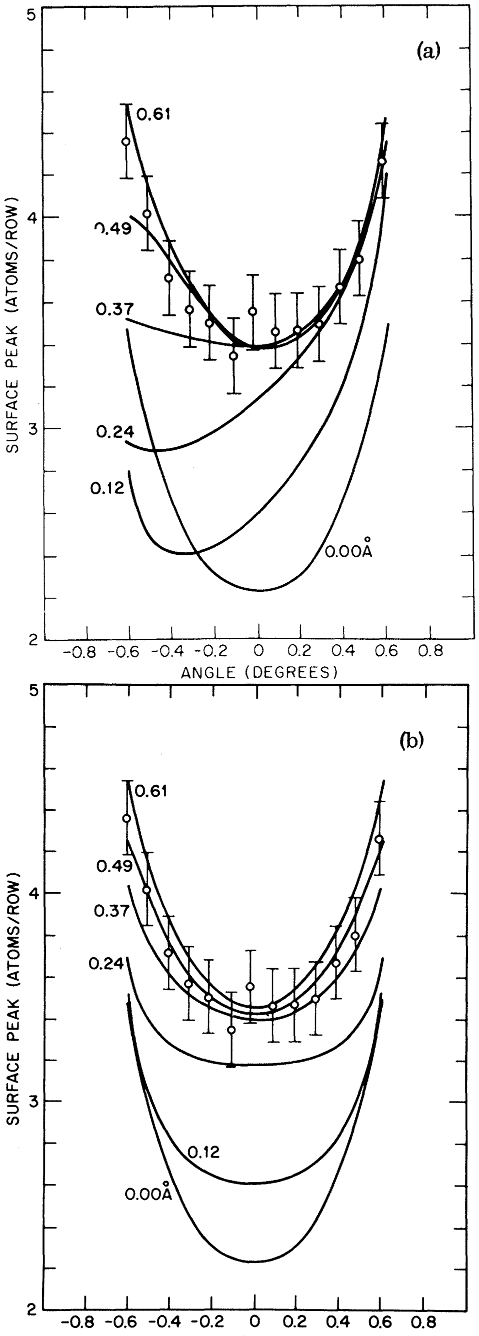

FIG. 3. Surface peak intensity as a function of tilt angle in the {110} plane for 500-keV He$^+$ incident in the ⟨001⟩ direction at 300 °K. The center of the experimental data was determined from bulk measurements obtained simultaneously. The calculated curves are from computer simulations with the first atoms of a string displaced perpendicular to the surface by the amounts indicated. The calculated curves in (a) are for the case of the first atom in the first two monolayers contracted while the curves in (b) result from the atoms in one monolayer contracted and the first atom in the second string relaxed.

ment (in the mean-square amplitude) of a factor of 4 in the first *two* monolayers of the surface (Fig. 2). Enhanced surface vibrations can have some effect on the quantitative interpretation of the data but clearly will not alter the main conclusion of this study, namely that the major reconstruction of the Si(111)-(7 × 7) surface involves substantial vertical displacements in two monolayers.

The interpretation of our experiments does not require a presumed model; general features of the surface structure are determined. While these results alone cannot explain the surface periodicity, any realistic model of the 7 × 7 structure[7] must incorporate the geometric features found here. The ⟨001⟩ data indicate that two layers have large displacements (~0.4 Å) normal to the surface. It is clear that this rules out any model with atoms in bulklike positions, such as a *pure* vacancy model.[8] Partial agreement is obtained with models having only perpendicular displacements, such as the rippled-surface model of Mark, Levine, and McFarlane,[9] which has a relaxation in the first two layers modulated by a small-amplitude ripple. The buckled-surface model of Chadi[10] contains both small parallel displacements and large perpendicular displacements in several layers. This type of model gives the best agreement with the present ion-scattering results. The epitaxial misfit strain model of Phillips[11] also involves lateral and normal displacements.

In conclusion, we have measured the SP intensity in the ⟨111⟩ and ⟨001⟩ directions for the Si(111)-(7 × 7) surface. The energy dependence of the ⟨111⟩ SP intensity is close to that expected for a bulklike structure and implies that transverse displacements are confined to one to two monolayers with a magnitude of $\lesssim 0.15$ Å. The angular dependence of the ⟨001⟩ SP intensity at 500 keV indicates that two monolayers have displacements of ~0.4 Å perpendicular to the surface. This provides the first definitive evidence that the major reconstruction in Si(111)-(7 × 7) involves large perpendicular displacements.

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Diffuse-X-Ray-Scattering Study of the Fast-Ion Conductor β-Ag_2S

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Disks of diffuse scattering are observed at $\vec{q} = \langle\sim 0.6, 0, 0\rangle$ around the bcc Bragg reflections implying correlations of the Ag ions in the [100] directions. The average correlation length and the inverse Haven's ratio both decrease with increasing temperature. The x-ray measurements provide structural evidence for strongly correlated ionic transport in β-Ag_2S.

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The mechanism for the high ionic conductivity in silver-based salts such as α-AgI is currently under active study.[1] The silver ions are highly disordered and can be treated as a "liquid" confined to the channels of the body-centered cubic lattice formed by the iodine ions. In β-Ag_2S, twice as many Ag ions are distributed in the channels of the bcc lattice of sulfur anions, and a caterpillar mechanism[2] for cooperative ionic charge transport has been proposed to explain the anomalously small ratio (Haven's ratio) of the diffusion coefficients derived from tracer and ionic