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Structure study of Si(111)-(7×7) by channeling and blocking

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The structure of the Si(111)-(7×7) surface has been studied by medium-energy ion channeling and blocking. From a comparison of experimental results of Monte Carlo calculations for a number of structural models we conclude that the models proposed by Bennett and by McRae and by Himpsel and Batra give reasonable to good agreement with experimental results.

Recently there has been an intensified effort to unravel the structure of the Si(111)-(7×7) surface.[1–11] Ion-channeling results indicate that atoms in the outer double layer do not shadow the underlying silicon lattice when viewed along an off-normal direction, but are close to bulklike sites when viewed along the normal.[1,2] Scanning tunneling microscopy (STM) has provided the first real-space image of the surface.[3] Per unit cell, 12 maxima and a large hole at the corner are observed, along with smaller minima at the sides of the cell. Whether these hills and depressions are due to atoms occupying lower and higher sites or to minima and maxima in the local electron density giving rise to a modulation of the tunneling current remains an open question.

The ion-scattering results posed a puzzle until Bennett *et al.*[4] proposed the presence of stacking faults to explain the peculiar direction dependence of the observed shadowing phenomena. In Bennett's model[5] the number of dangling bonds in the surface is reduced by the absorption of 12 adatoms per (7×7) cell. The strain induced by these adatoms is partially relieved by the presence of stacking faults, dividing the unit cell in two triangular areas.[5] McRae proposed a similar stacking-fault model which explains the channeling results and the depressions observed in the STM experiment.[6] The maxima in the STM picture are thought to be caused by special surface states. Himpsel and Batra have proposed a model involving a stacking fault and a rebonding in the surface.[7] Twelve atoms per (7×7) cell rebond in the same way as the atoms in the π-bonded chain model proposed by Pandey[8] for the Si(111)-(2×1) surface. Instead of infinite chains these 12 atoms form trimers of atoms with their neighbors. The surface energy is thought to be reduced by π bonding in these trimers. Snyder has proposed a modification of his "milk stool" model,[9] which Aono, Souda, Oshima, and Ishizawa[10] independently found on the basis of their low-energy-ion scattering (LEIS) studies. This "pyramidal cluster" model consists of 12 clusters of 4 atoms each, adsorbed on the surface as pyramids and arranged within the unit cell to fit the pattern of maxima observed in the STM image. Assuming sp^3 bonding in these clusters, the unit cell contains 97 dangling bonds instead of 49, but this number is lowered by sp^2 hybridization.[9] Nevertheless, total-energy calculations performed by Northrup and Cohen indicate that the total energy per surface atom is higher than that of the bulklike surface by 0.5 eV.[11] The same total-energy calculations[11] indicated that adatoms may possibly explain the (7×7) structure and the STM image, just as Binnig, Rohrer, Gerber, and Weibel[3] originally interpreted their result.

In this study we have measured surface blocking minima[14] on the Si(111)-(7×7) surface (using the ion-scattering equipment at the FOM–Institute in Amsterdam) and compared experimental results with the structural models discussed above. Figure 1 shows experimental results obtained with 98.6-keV protons in the geometry shown in the inset. The number of atoms per row visible to ion beam and detector (plotted as function of scattering angle) is very sensitive to static displacements of atoms in the surface from a bulklike position. If such displacements (static or dynamic) are absent, the first atom in each $[00\bar{1}]$ row will shadow subsurface atoms and only the first atom in each $[00\bar{1}]$ row is visible to the ion beam: the number of atoms per row is equal to 1. Static and/or dynamic displacements

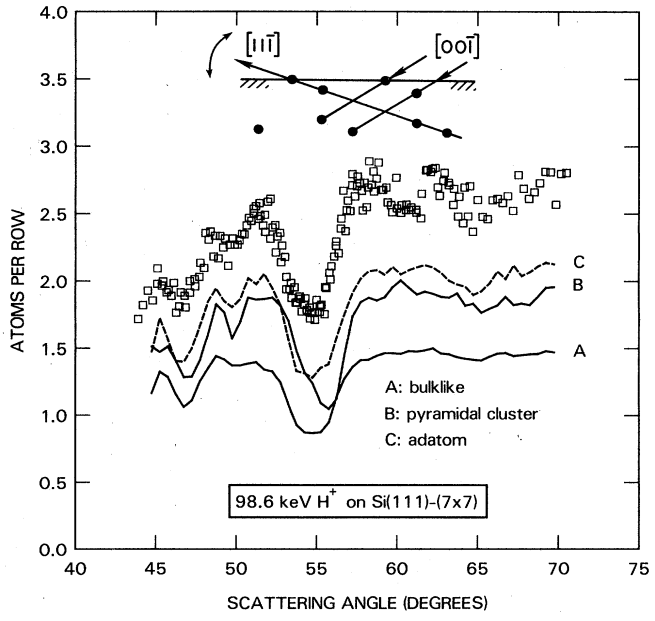

FIG. 1. Comparison of experimental results with various structure models discussed in the text. The scattering geometry is shown in the inset.

will reduce the effectiveness of the shadowing and give rise to an increase in the number of atoms per row. Along the outgoing [11$\bar{1}$] direction (at a scattering angle of 54.74°) the number of atoms per row is reduced due to blocking of ions scattered below the surface by atoms closer to the surface. Similar blocking effects occur along higher index directions, giving rise to a number of additional surface blocking minima. Since the ion-target collisions at the energies used in this study (50–150 keV) are classical elastic collisions and since the cross sections are accurately known, the experiment can be simulated in a computer by a Monte Carlo procedure[12,13] for any desired crystal structure. A given unit cell is repeated by periodic boundary conditions parallel to the surface and the track of the ions through this crystal is followed.[13] The result of such simulations can be compared quantitatively with experimental results.[14]

The solid line (a) in Fig. 1 is the result of such a simulation for a bulklike surface: bulklike positions and bulklike thermal vibration amplitudes (0.078 Å one-dimensional rms) are assumed for all atoms. The measured number of atoms per row is higher than this calculated curve by about one atom per row, corresponding to two monolayers (1 ML $= 7.83 \times 10^{14}$ atoms/cm^2), indicating that the outer Si double layer does not shadow the underlying crystal, in good agreement with earlier results.[1,2]

The solid line (b) is the result for the pyramidal cluster model as specified by Snyder.[9] This includes relaxations from "ideal" positions due to rehybridization of the pyramid atoms. If such relaxations are not taken into account the simulations result in a curve very close to that for the bulklike surface. If the surface underneath the pyramids contains a stacking fault, consisting of a monolayer of Si rotated over 60° (a single wurtzite layer), the number of atoms per row increases. However, the shape of the blocking curve is very different from the experimental results.[15] Thus, the pyramidal cluster model is inconsistent with our results.

This rejection of the pyramidal cluster model seems to present an inconsistency with the low-energy-ion scattering results by Aono *et al.*[10] The basic observation in this LEIS study was the presence of scattering centers, roughly 8 Å apart. We note that such scattering centers are present in models having one or two different stacking faults within the surface unit cell, giving rise to a large hole at the corner and smaller holes along the sides of the unit cell. These holes create a large local surface roughness where ions can be scattered over a large angle, even at a small angle of incidence. Although the presence of these holes may be insufficient to explain the results by Aono *et al.*, they form an important contribution in models less rough than the pyramidal cluster model. In order to address this question in more detail Monte Carlo simulations must be performed for Aono's experiment in a full (7×7) unit cell. Such an analysis is complicated by uncertainties about the charge state of the particles reflected into the vacuum.

Line (c) (dashed) was calculated for the adatom model as it was proposed by Harrison[16] and adapted by Binnig *et al.*[3] As has been pointed out by Northrup and Cohen,[11] in considering the adatom model, subsurface relaxations induced by the adsorption of the adatoms have to be taken into account. We did this by minimizing the total elastic energy in the outer six layers of the crystal by a Keating-type calculation.[17,18] For an adatom in a (2×2) geometry we compared results from a self-consistent pseudopotential calculation[11] with results obtained with the Keating calculation and found them to be very similar, as far as atomic positions and calculated surface blocking minima are concerned.[15] Thus, we have also applied these Keating calculations to Binnig's model. The increase we observed from line (a) to line (c) is entirely due to these strain-induced relaxations. If these are not taken into account, the adatom model and the bulklike surface give almost the same surface blocking minimum.[15]

The results for the models by Bennett, McRae, and Himpsel and Batra are shown in Fig. 2.

Line (a) was calculated for Bennett's model.[5] The positions of the adatoms and of the atoms in the outer three double layers were optimized to minimize the elastic strain in the surface.

Line (b) was calculated for McRae's model.[6] Again, the coordinates in the outer six layers have been optimized to reduce the elastic strain energy. In this case the difference between the relaxed and the unrelaxed structure is small, but the relaxed structure gives better agreement with the experiment.[15]

Finally, line (c) is the result for the trimer model by Himpsel and Batra.[7] In this model subsurface displacements are rather large. The structure is optimized by minimizing the elastic energy. Different values for the Keating constants were tried, but the blocking curves are rather insensitive to the values chosen.[15] The coordinates in five layers were optimized.

The results for these three models are very close to each other. For the models by Bennett and McRae this is not unexpected, since they are very similar, both having stacking faults in the outer two double layers as a main feature. These stacking fault models agree well with the experimental results. The trimer model gives equally good agreement, although it is a rather different model, having a stacking

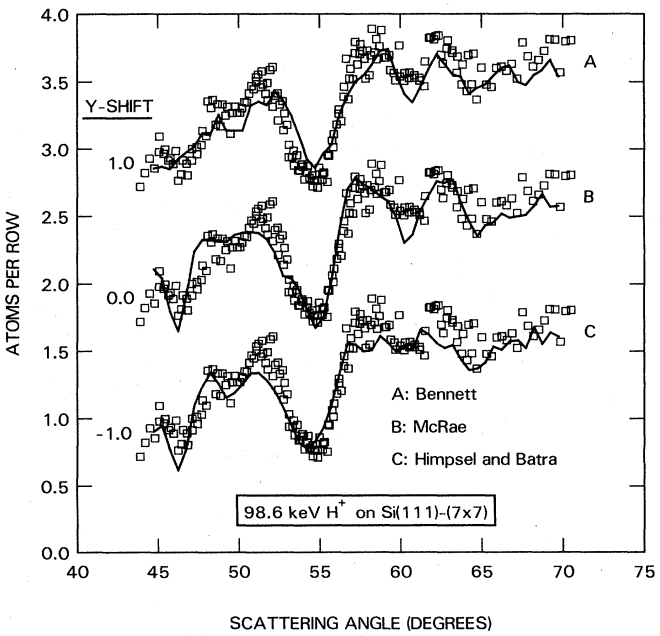

FIG. 2. Comparison of experimental results with various structure models. Data and calculations have been shifted in the Y direction as indicated.

fault in half of the outer double layer only. We have also considered other ion energies and other backscattering geometries and reach the same conclusions.[15] We are not able to distinguish between these models with the present ion-scattering results. Evidently, this leaves open the possibility that other models may be conceived that give similar agreement with the experimental results presented here. Nevertheless, we consider the exclusion of some of the models presently being considered an important step in the analysis of the structure of the Si(111)-(7×7) surface.

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