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Low-Energy Electron Diffraction Determination of the Atomic Arrangement on Impurity-Stabilized Unreconstructed Si{111} Surfaces

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An impurity-stabilized Si{111} 1×1 structure has been obtained by depositing minute amounts of Te on a clean Si{111} 7×7 surface. A low-energy electron diffraction structure analysis of this 1×1 structure reveals that the atomic arrangement is essentially bulklike, but involves a slight contraction of the first interlayer spacing by about 15% with respect to the bulk value.

It is a matter of considerable interest that, despite the great deal of attention that has been devoted to Si surfaces in recent years, no direct determination has been made of the atomic arrangements on such surfaces. The problem of acquiring such knowledge is complicated by the fact that at least the three lowest index surfaces of Si (i.e., the {001}, {110}, and {111} surfaces) in their clean state have structures different from those of the equivalent bulk planes or, in the language of surface crystallography, are "reconstructed." The Si{001} surface, for example, exhibits a so-called 2×1 structure, the periodicity in one of the ⟨110⟩ directions on the surface being twice as large as the one on bulk {001} planes. The vacuum-cleaved Si{111} surface also exhibits a 2×1 structure, but the annealed Si{111} surface exhibits a 7×7 structure, which has a unit mesh 49 times larger than a bulk {111} plane. The electronic structures of both Si{001} and Si{111} surfaces have been objects of extensive experimental[1-8] and theoretical[9-14] investigations, while the corresponding atomic structures have only been objects of sophisticated speculations.[15-21]

In recent years, a great deal of effort has been devoted to the study of the Si{001} 2×1 structure by several of the groups active in LEED (low-energy electron diffraction) crystallography,[22-26] but no solution of the problem has yet been reported. One of the most puzzling aspects of this failure has been the unanswered question about the basic capability of either the multiple-scattering or the data-averaging methods used in LEED crystallography[27] to treat the diamond lattice properly and accurately. Legitimate questions have been raised, in particular, about the correctness of the muffin-tin model for the description of the Si lattice.

Somewhat less attention has been devoted to the atomic structure of the Si{111} surface, probably because the 2×1 superstructure requires *in situ* cleaving of a Si single crystal (not a universally available facility) and the 7×7 superstructure is just too complicated to handle at the present time. However, Florio and Robertson[28] established a few years ago that the Si{111} 7×7 structure reversibly transforms into a 1×1 structure at 900°C and that the 1×1 structure can be "impurity-stabilized" by minute amounts of Cl on the surface at room temperature. Hagstrum and Becker[29] reported that the 1×1 structure can be quenched on the clean Si{111} surface by rapid cooling from

830°C. Either the quenched or the impurity-stabilized Si{111} 1×1 structure appears to be a much more promising candidate for LEED structure analysis than any of its reconstructed counterparts. Firstly, a 1×1 structure is computationally easier to handle than either a 2×1 or a 7×7 structure. Secondly, the analysis of such a 1×1 structure, if successful, would provide a long-awaited answer to the question about the ability of present LEED crystallographic procedures to treat the diamond lattice correctly. Thirdly, the knowledge of the atomic arrangement on Si{111} 1×1 would likely yield useful guidelines for the solutions of the more complicated structural problems of Si{111} 2×1 and Si{111} 7×7. For these reasons we have undertaken the project of preparing a Si{111} 1×1 surface, collecting the LEED intensity data, and carrying out a structure analysis. We report herein the first successful results of this analysis.

The Si sample was cut from a commercially available, polished, 20-Ω-cm, *p*-type wafer.[30] After suitable ion bombardment and annealing, the {111} surface exhibited the well-known 7×7 superstrucutre. Auger electron spectroscopy (AES) revealed, as usual, the presence of C, the ratio of differentiated C line at 274 eV to Si line at 92 eV being typically 2.5×10^{-3}. This surface was then exposed to a beam of Te vapor in an ambient of 10^{-10} Torr. At room temperature, the deposited Te film was amorphous, while gentle heating to about 500°C produced a $(2\sqrt{3}\times2\sqrt{3})$-30° superstructure. Prolonged heating to higher temperatures eventually caused Te to disappear and reconstituted the clean 7×7 structure, but prior to this a 1×1 structure was observed. AES of this 1×1 structure revealed the presence of Te on the surface—in the differentiated AES spectrum, the ratio of the intensity of the Te line at 485 eV to that of the Si line at 92 eV was smaller than 1×10^{-3}. By comparing this ratio to that observed for the Si{111} $(2\sqrt{3}\times2\sqrt{3})$-30°-Te structure and assuming a surface coverage no larger than $\frac{1}{3}$ for the latter, we estimated that the concentration of Te on the 1×1 surface was less than 5%, and probably as low as 1%, of one monolayer. Thus, the 1×1 structure was indeed an impurity-stabilized structure. We eventually developed three different procedures for the preparation of this Te-stabilized Si{111} 1×1 structure, viz. (i) deposit about one monolayer-equivalent of Te on the 7×7 structure at about 1000°C, stop the deposition, and cool very rapidly; (ii) deposit at least one monolayer-equivalent amount of Te on the 7×7 structure at room temperature, heat to about 900°C for 2–3 sec, and then cool rapidly to room temperature; (iii) obtain the Si{111} $(2\sqrt{3}\times2\sqrt{3})$-30°-Te structure, and then sweep the surface with a 3-keV, 0.3-mA electron beam (e.g., with the AES gun) for about 5 min.

Eleven LEED spectra at two different angles of incidence were collected with the conventional spot-photometer technique from both a surface prepared with procedure (i) and a surface prepared with procedure (iii). Corresponding spectra from either surface are, of course, equal. We present here those collected from a surface prepared with procedure (iii). LEED intensity calculations were carried out with the layer-KKR (Kohn-Korringa-Rostoker) procudure[31] using 61 beams and eight phase shifts to describe the electron wave function. Calculations done with 85 beams produced spectra with identical curve shapes. The real part of the Si potential used was a muffin-tin potential produced from superposition of atomic charge densities[32]; the imaginary part was 3.0 eV and the inner potential was 9.0 eV. No Te was assumed to be present on the surface in the calculations. We found excellent agreement between the observed and calculated spectra for a relaxed truncated-bulk model of the Si{111} surface in which the first interlayer spacing was $d_z^S = 0.66$ Å (bulk value $d_z = 0.78$ Å), i.e., contracted by about 15% with respect to the bulk value. Curves calculated for a contraction of 0.3 Å in d_z^S (≈38% with respect to the bulk value) are in strong disagreement with experiment. We present, in Fig. 1, four examples of the kind of correspondence between observations and calculations that we have obtained for all eleven beams tested. The dashed curves correspond to the unrelaxed surface, the solid theoretical curves to 15% contraction. We note that some beams are more sensitive than others to changes in the interlayer spacing—a well-known fact in LEED crystallography. Of the beams shown in the figure, the "20" beam at $\theta = 0°$ and the "00" beam at $\theta = 8°$ are rather insensitive, whereas the "11" beam at $\theta = 0°$ and the "$\bar{2}$1" beam at $\theta = 8°$ are quite sensitive to d_z^S and clearly favor the relaxed surface. We expect that refinement of both the structural and the nonstructural parameters will improve the correspondence even further.

We believe that the solution of this particular structural problem is significant for a number of reasons. In the first place, since it was reported by Florio and Robertson[28] that the impurity-stabilized 1×1 and the high-temperature 1×1 phase

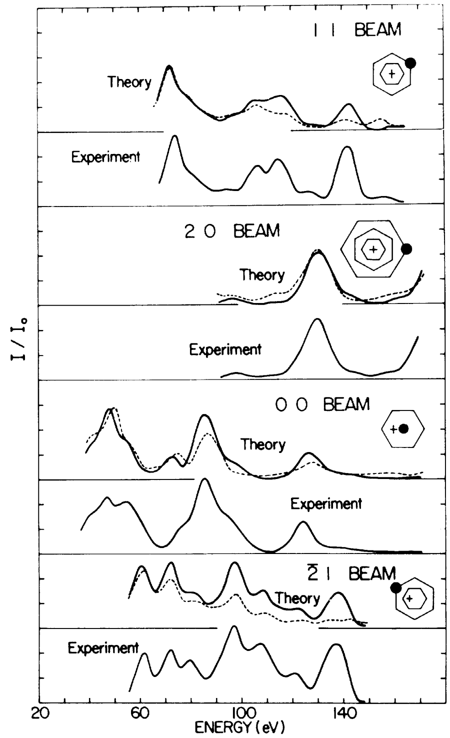

FIG. 1. Comparison between the observed and calculated spectra for the impurity-stabilized Si{111} 1×1 surface: "11" and "20" beams at normal incidence; "00" and "$\bar{2}1$" beams at $\theta = 8°$ and $\varphi = 0°$. The dashed curves were calculated for an unrelaxed surface, the solid (theoretical) curves, for a 15% contraction of the first interlayer spacing. In each panel, the hexagon represents schematically the observed LEED pattern, the full circle indicates the position of the tested beam, and the cross shows the position of the electron gun on the screen.

of the clean surface are probably the same structure, our result establishes that the clean Si{111} 1×1 surface is essentially bulklike, i.e., involves little distortion of the bulk structure. In the second place, the very fact that the problem could be solved confirms the reliability of the layer-KKR procudure in dealing with the diamond lattice. In particular, it establishes the validity of the muffin-tin potential for electron scattering at LEED energies, despite the strongly covalent bonding in the diamond lattice. Finally, there is a clear indication that more studies of the electronic structure of impurity-stabilized Si{111} 1×1 surfaces would be fruitful at this time. There is, in fact, a discrepancy between the results of different techniques. Best,[6] on the one hand, reported noticeable differences between the angle-resolved secondary-electron-emission spectra of the 7×7 and 1×1 structures; Pandey, Sakurai, and Hagstrum,[33] on the other hand, reported very similar photoemission spectra from either surface; and the observations of Florio and Robertson[28] (and our own) show that the corresponding LEED spectra of the 1×1 and 7×7 structures are not very different from one another.

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Macroscopic Calculation of the Kapitza Resistance between Solids and Liquid ^{4}He

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We treat the Kapitza thermal boundary resistance R_K between a Debye solid and liquid ^{4}He in the temperature range 0.1 to 1 K, where the phonon transmission coefficient is known to be highly anomalous. Using a continuum model, we consider the consequences of a solid van der Waals layer of helium which is acoustically absorbing. Using values of acoustic wave attenuation in the layer based on experiment, we are able to predict the correct order of magnitude and temperature dependence of R_K for copper.

The anomalously high phonon transmission coefficient between liquid helium and solids has been a well-known problem since its discovery by Kapitza in 1941.[1] Khalatnikov[2] proposed an acoustic mismatch model which in its simplest form failed to predict the observed magnitude of the effect.[3] In this Letter we propose a more general macroscopic model based on acoustic mismatch which successfully predicts the order of magnitude of the experimental results.

The Kapitza effect has been found to exist[4,5] in both liquid and solid ^{3}He and ^{4}He and even solid H_2 and D_2 and it is now generally believed to be characteristic of quantum systems. For simplicity and brevity we restrict our discussion here to the "classic" problem of the steady-state thermal boundary resistance R_K for phonon transport between an isotropic ordinary Debye solid in contact with a bath of liquid ^{4}He in the temperature range 0.1 to 2 K. In this case classic acoustic theory predicts the existence of a small critical cone for total reflection in the helium as a result of the large difference in acoustic properties of the two media. The small transmission coefficient for incidence within this cone explains the high values of R_K predicted by the Khalatnikov theory.

A first attempt to provide a mechanism for an increased phonon transmission coefficient was made by Challis, Dransfeld, and Wilks (CDW),[6] who took into account the formation of a dense layer of helium at the interface due to the van der Waals attraction of helium atoms to the substrate. This layer acts as an acoustic matching unit which leads to an increased transmission coefficient within the critical cone; this is, however, quite insufficient in itself to resolve the discrepancy. More recently, other workers[7,8] have considered the effects of a finite phonon lifetime in the substrate, which led to an effective widening of the critical cone. The two mechanisms have been combined in a single calculation by Opsal and Pollack.[9] However a large body of evidence[10] suggests that substrate lifetime effects cannot provide the sole basis for the correct explanation for $T \gtrsim 1$ K and we do not consider them further here.

The present model uses the existence of a