In conclusion, we have found excess linear dissipation in $B$-phase flow at saturated vapor pressure persisting to the lowest measured velocities. The mechanism of the dissipation is unknown. Although some purely classical effect could be the cause, a review of past flow measurements reveals no convincing evidence of dissipationless $B$-phase flow. The basic nature of the question this raises about our understanding of superfluid $^3$He suggests further effort, both theoretical and experimental.

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# Low-Energy Ion Scattering from the Si(001) Surface

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The structure of a clean Si(001) surface has been studied by a specialized technique in low-energy ion scattering spectroscopy. It has been found that (1) the surface is dimerized, and (2) the intradimer atomic distance parallel to the surface is $2.4\pm 0.1$ Å.

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The clean annealed Si(001) surface is reconstructed into a $(2\times 1)$ structure[1-4] with substantial subsurface strain,[5] although a $c(4\times 2)$ structure coexists in a small proportion.[6-8] Concerning this surface reconstruction, many models, e.g., vacancy models,[7,9,10] conjugated-chain-type models,[4,11] and dimer models,[1,2,12-14] have been proposed, but comparisons of calculated surface electronic structures[14-16] for the various models with photoemission data[17,18] suggest that the dimer models are the most favorable. In this Letter, we report that (1) the surface is certainly dimerized, and (2) the intradimer atomic distance parallel to the surface is $2.4\pm 0.1$ Å. These results have been obtained by a specialized technique[19] in low-energy (of order kiloelectronvolts) ion scattering spectroscopy (ISS),[20] which we call impact-collision ion scattering spectroscopy (ICISS).[19] The specialization used in ICISS is to take the experimental scattering angle $\theta_L$ at 180° (or close to 180°) so as to observe such scattered ions as have made head-on collision (or impact collision) against target atoms with zero (or nearly zero) impact parameter $b$. Despite its simplicity, this specialization yields useful new aspects as described elsewhere.[19]

A Si(001) sample with a diameter of 10 mm and a thickness of 0.2 mm was treated according to a prescription reported by Henderson.[21] The sample was mounted on a manipulator by means of thin tantalum wires with care taken to minimize mechanical stress, and cleaned/annealed *in situ* (base pressure ~ $5\times10^{-11}$ Torr) by electron-beam heating (~1250 °C) from behind. The sample exhibited a clear (2×1) diffraction pattern in low-energy electron diffraction (LEED); no $c(4\times2)$ pattern was visible with our LEED optics in accordance with many other reports.[1-4] Experiments of ICISS were done using $He^+$ ions of 1 keV (~20 nA/cm$^2$) and an electrostatic energy analyzer in a similar way to that reported elsewhere.[19] During the experiments, the sample was annealed at appropriate time intervals.

Figure 1 shows the intensity of $He^+$ ions scattered from the Si(001) surface in the ICISS condition as a function of polar angle $\alpha$ (measured from the surface) and azimuth angle $\varphi$ (measured from [110]) of the ion incidence direction. The intensity variations seen in Fig. 1 are due to two effects: One effect is that the probability of ion neutralization[20] in ion scattering by solid surfaces, which is very high (~100%) for low-energy ions, depends on $\alpha$ and $\varphi$, although the $\varphi$ dependence is usually weak; and the other effect is a shadowing effect[20] such that an atom in an ion beam forms a shadow called a shadow cone[22] in which incident ions cannot penetrate, and if an atom is concealed by this shadow cone at certain $\alpha$ and $\varphi$, this atom has no contribution to ion scattering. In conventional ISS, a blocking effect,[23] in which a scattered ion may be blocked by another atom, must also be taken into account, but this troublesome effect never occurs in ICISS since ions backscattered along their incident trajectories are selectively observed because of $\theta_L = 180°$. In this Letter, we analyze the shadowing effect for determining surface atomic geometry. In the ICISS condition, the analysis of the shadowing effect is simple since at a critical angle corresponding to the onset of the shadowing effect, the edge of the shadow cone necessarily passes the center of a concealed atom to a good approximation[19] because of $b = 0$.

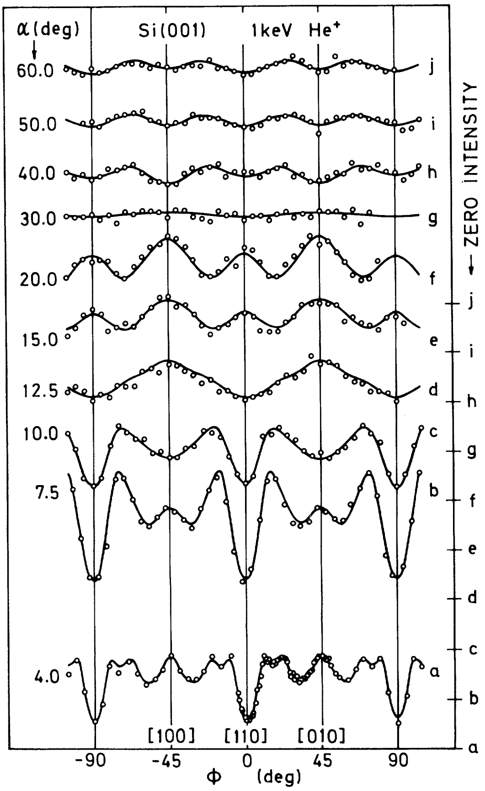

FIG. 1. The intensity of $He^+$ ions scattered from Si(001) in the ICISS condition as a function of polar angle $\alpha$ (measured from the surface) and azimuth angle $\varphi$ of the ion incidence direction.

By virtue of the high ion neutralization probability[20] mentioned above, ICISS (and conventional ISS) is highly sensitive to the surface first layer, and hence shadowing effects which occur within the first layer at grazing angles are observed most markedly. The intensity curve for a grazing angle of $\alpha = 4°$ in Fig. 1 is magnified in part in Fig. 2. The intensity drops at $\varphi = 0°$ ([110]), 32 ± 1° (azimuth $S$), and 58±1° (azimuth $S'$) are unambiguously identified to be due to shadowing effects since an intensity rise due to a focusing effect,[22] that ion flux is necessarily concentrated just outside a shadow cone, is clearly observed on the both sides of the individual intensity drops as indicated by broken curves. The dash-dotted line shows the reference intensity that is expected when both the shadowing and focusing effects are assumed to be absent: This reference intensity is somewhat amibguous since the ion neutralization probability varies with $\varphi$, but the variation is ~± 6% at most as estimated from the intensity curves for high $\alpha$'s in Fig. 1 for which no marked shadowing effect is expected. In Figs. 1 and 2, the intensity drops due to the shadowing effects are observed with half widths of ~10–14°, from which the radius of the shadow cone of Si at ~4 Å, for example, from the center of the Si atom is estimated to be ~0.7–1.0 Å (for 1-keV $He^+$).

The dimer models[1,2,12-14] are classified into

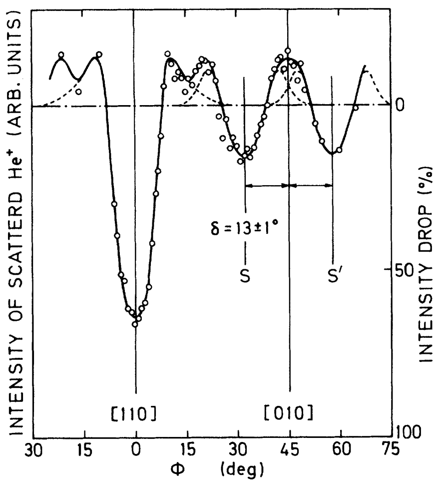

FIG. 2. The intensity curve for $\alpha = 4°$ in Fig. 1 magnified in part. The intensity drops at $\varphi = 0°$, $32 \pm 1°$, and $58 \pm 1°$ are due to shadowing effects.

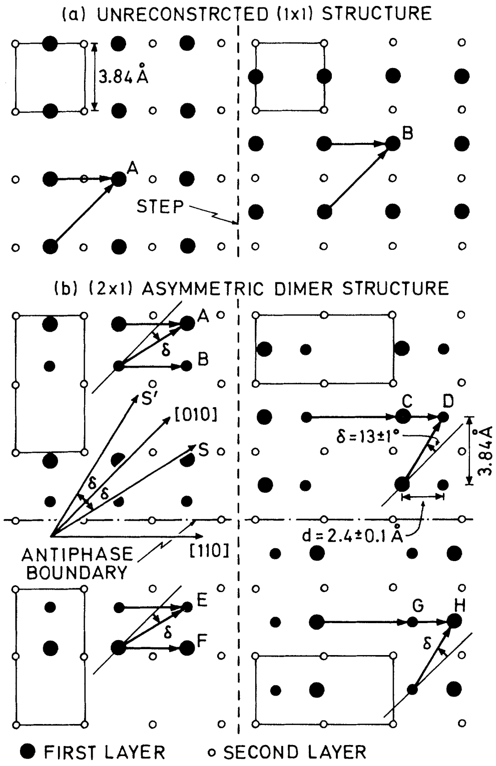

FIG. 3. (a) The unreconstructed $(1\times 1)$ structure, and (b) the $(2\times 1)$ asymmetric dimer structure of Si(001).

"symmetric"[1,2,12,13] and "asymmetric"[14] dimer models. The symmetric dimer model was studied theoretically by Appelbaum and Hamann.[13] They found that the stress due to the formation of the symmetric dimers at the surface can produce substantial subsurface strain. This is consistent with recent high-energy He$^+$ ion-scattering experiments.[5] However, the symmetric dimer model is inaccurate since this model yields a metallic surface[15,16] which disagrees with photoemission data.[18] Furthermore, the symmetric dimers can form only a $(2\times 1)$ structure because of their twofold symmetry, whereas actually a $c(4\times 2)$ structure is observed in a small proportion in addition to a $(2\times 1)$ structure by LEED[6,7] and He-atom diffraction.[8] Using energy-minimization calculations, Chadi[14] found that the symmetric dimer model is unstable; the total energy is lowered by the formation of *asymmetric* dimers (and by subsurface distortions like those described by Appelbaum and Hamann[13]). The asymmetric dimers can form both $(2\times 1)$ and $c(4\times 2)$ structures depending on their in-phase and out-of-phase arrangements, respectively,[14] and yield semiconducting surfaces.[14] Figure 3(b) shows the in-phase arrangement of the asymmetric dimers which results in a $(2\times 1)$ structure consistent with our LEED observation, and for comparison the unreconstructed $(1\times 1)$ structure is shown in Fig. 3(a). In the figures, the solid circles show atoms in the first layer, and the broken line indicates a step which divides the surface into two kinds of terraces which are rotated relative to each other by 90°; in Fig. 3(b), the dash-dotted lines show antiphase boundaries which divide the individual terraces into two kinds of domains, and the large and small solid circles indicate the "up" and "down" atoms of the asymmetric dimers, respectively. The number of surface atoms not equivalent in view of ion scattering is two ($A$ and $B$) in Fig. 3(a) and eight ($A$–$H$) in Fig. 3(b).

Figure 2 contains the following information: (i) The shadowing effects are observed in [110] and in azimuths $S$ and $S'$ which deviate from [010] by $\delta = 13 \pm 1°$, and (ii) the magnitudes of the intensity drops due to the shadowing effects relative to the reference intensity are $\Delta I([110]) \simeq 63\%$ and $\Delta I(S \text{ or } S') \simeq 15\%$. On the basis of these experimental facts (i) and (ii), we can discuss the structure of the Si(001) surface as follows. In the following discussion, we will consider the case of $\alpha = 4°$ corresponding to Fig. 2, and the radius of the shadow cone of Si mentioned above will be taken into consideration. As expected, the unreconstructed $(1\times 1)$ structure, Fig. 3(a), is rejected since shadowing effects for this structure should occur in $\langle 110\rangle$ and $\langle 010\rangle$ as indicated by arrows in contradiction to the experimental fact (i). The experimental fact (i) indicates that the surface is dimerized like Fig. 3(b); in this case, as indicated by arrows, shadowing effects occur in [110] and in azimuths which deviate from [010] by some angle $\delta$ in agreement with the experimental fact (i). At $\alpha = 4°$ of concern, eight surface atoms ($A$–$H$) are all concealed in [110], while only $A$ and $E$ (or $D$ and $H$) are concealed in azimuth $S$ (or $S'$). That is, the magnitude of the intensity drop in [110] should be larger than that in azimuth $S$ or $S'$ by a factor of 4. This agrees well with the experimental fact (ii), i.e., $\Delta I([110])/\Delta I(S \text{ or } S') \simeq 4.2$. In Figs. 1 and 2, and we find the following additional experimental facts: In Fig. 1, as $\alpha$ decreases, the shadowing effect in [110] begins first, and that in azimuths $S$ and $S'$ begins after that (the critical value of $\alpha$ at which a shadowing effect begins depends on the distances parallel and perpendicular to the surface between the shadowing and concealed atoms), and in Fig. 2, the magnitude of the intensity rise due to the focusing effect relative to that of the intensity drop due to the shadowing effect is larger for azimuths $S$ and $S'$ than for [110] (in general, this ratio increases with increasing linear distance between the shadowing and concealed atoms since ion flux just outside the shadow cone of an atom is concentrated more remarkably as the distance from the atom increases). By examining Fig. 3(b) we find that these additional experimental facts are also consistent with Fig. 3(b). From the experimental fact (i), $\delta$ in Fig. 3(b) is $13 \pm 1°$, which means that the intradimer atomic distance parallel to the surface is $2.4 \pm 0.1$ Å. A corresponding theoretical value calculated by Chadi,[14] 2.3 Å, agrees well with this experimental value.

It is known that even if only a $(2\times1)$ diffraction pattern is observed in LEED as in the present experiment, He-atom diffraction[8] reveals the coexistence of a $c(4\times2)$ structure; this indicates that the $c(4\times2)$ structure, which is thought to be formed by the out-of-phase arrangement of the asymmetric dimers,[14] exists as small domains whose dimension is smaller than the coherent length of LEED (but larger than that of He-atom diffraction). In one of the two kinds of terraces (cf. Fig. 3), adjacent surface atoms in the $c(4\times2)$ structure are not lined up along [110] (not shown). The reason why the intensity curve in Fig. 2 does not drop to zero in [110] in disagreement with the estimation for Fig. 3(b) at $\alpha = 4°$ can be attributed in part to the existence of the $c(4\times2)$ structure, although the steps and antiphase boundaries as well as other defects, including disordered areas, also contribute to the nonzero intensity.

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