Effect of electric current on the ratio of the areas of the (2×1) and (1×2) domains at the clean (001) surface of silicon during sublimation

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A part of the surface occupied by the domains with a (2×1) or (1×2) structure at an atomically pure (001) surface of silicon is found to depend on the direction and magnitude of the electric current which heats the crystal.

The atomically pure (001) surface of silicon is known to contain superstructural (2×1) and (1×2) domains. Reconstruction at Si(001) is contingent upon a dimerization of atoms, which have two broken bonds each, along the ⟨110⟩ direction involving the formation of the (1×2) superstructure. In the next atomic (001) plane, which lags behind the preceding plane a distance of $a/4$, the direction of dimerization changes by 90° and a (2×1) superstructure forms on it. If the steps of monatomic height ($a/4$) include the surface, the adjacent terraces will have different superstructures. If, however, the height of the steps is $a/2$, the same superstructure, (1×2) or (2×1), will form on all terraces.[1–7]

In this letter we report the results of an experimental study of the structural changes that occur at the (001) $\pm 2'$ surface of silicon. The results were obtained by an *in situ* method under a reflection electron microscope in an ultrahigh vacuum.[8] The test crystals were heated by passing an electric current (ac or dc) through them.

After removing the impurities (at 1250 °C for 10 min) the surface of silicon had a regular system of monatomic ($a/4$) steps. At $T > 800$ °C the test crystal is sublimated. During this process, the steps are the source of adatoms which are desorbed at the surface. As a result, the steps are displaced in the direction determined by the initial disorientation of the sample.

If the crystal is heated by an alternating current, a system of uniformly spaced monatomic steps, which move during the sublimation without changing their relative spacing, is formed at the clean surface. The terraces between the steps have alternately light and dark contrasts (Fig. 1a) because of the alternation of the (1×2) and (2×1) superstructures at $a/4$ step height (see Fig. 2a).

Sublimation of the crystal under direct-current heating conditions of the sample at $T > 900$ °C leads to a pairwise convergence of the monatomic steps. A minimum spacing of the steps in the pair reaches 0.1 μm when the average spacing in the

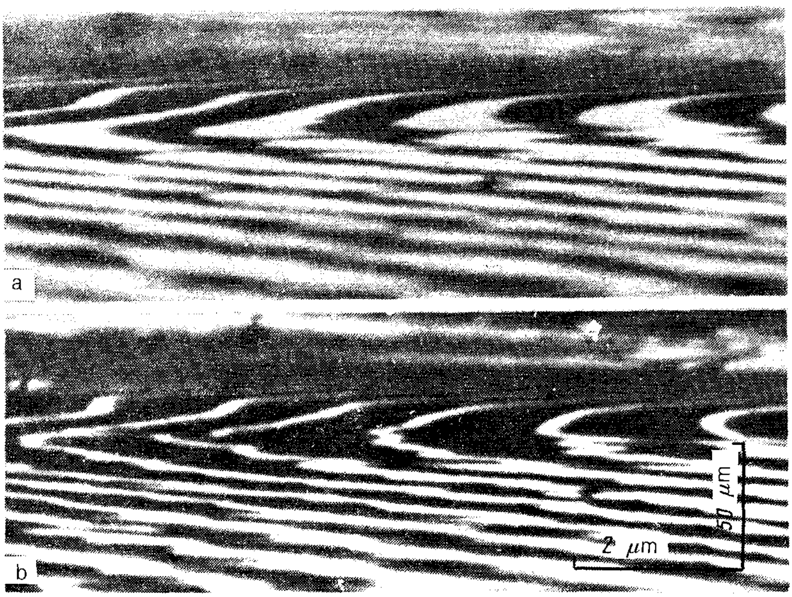

FIG. 1. Reflection-electron-microscope imaging of the same section of an atomically pure (001) surface of silicon, obtained in a superstructural (1×2) reflection, with the electron beam directed in the ⟨110⟩ direction. This section shows a system of uniformly spaced monatomic steps when it is heated with a 50-Hz alternating current (a). The (2×1) domains are dominant when the section is heated by a direct electric current whose flow is in the same direction as that of the motion of monatomic steps in the course of sublimation (b). The regions of elevated intensity are the image of the surface with a (1×2) superstructure and the regions of lowered intensity represent the (2×1) superstructure. The regions with different contrasts are divided by monatomic steps of height $a/4$.

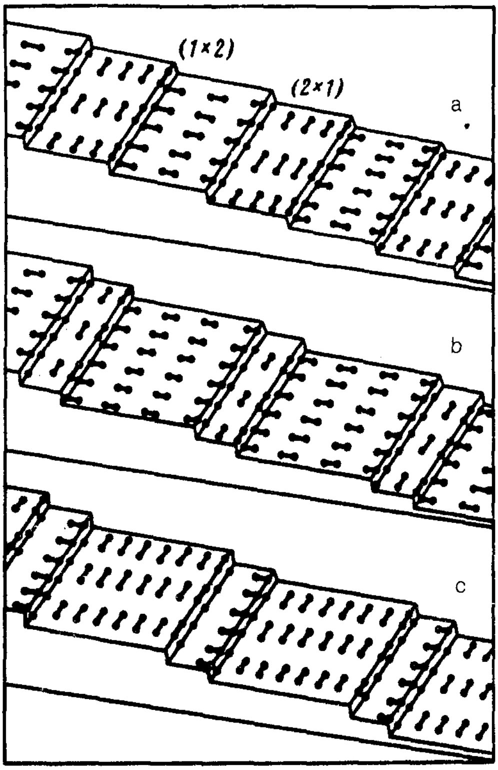

FIG. 2. Schematic diagram of the structure of the (001) surface of silicon in the course of the sublimation upon heating with an alternating current (a) and with a direct current. The direction of the direct current flow, indicated by the arrow, is opposite (b) or the same (c) as that of the motion of monatomic steps in the course of sublimation in the case under consideration.

equidistant system is 0.5–2 μm. If the direct current flows in the direction opposite that of the motion of the steps during sublimation, then nearly the entire surface will have a (1×2) superstructure: The dimers are perpendicular to the monatomic steps and the spaces between the steps in the pair are characterized by the (2×1) superstructure—the dimers are parallel to the steps (Fig. 2b). If the direction of the current and the steps is the same, the surface has primarily a (2×1) superstructure (Figs. 1b and 2c).

Transition from one type of surface to another as a result of the reversal of polarity of the direct current is reversible. This transition is brought about by reducing the velocity of the lower step in the given pair and increasing the velocity of the upper step during the sublimation. At temperatures below 900 °C a system (of the type shown in Fig. 1a) of uniformly spaced monatomic steps with alternating (1×2) and (2×1) superstructures on the terraces is stable, regardless of the direction in which the direct current flows.

It may be assumed that the ratio of the parts of the surface occupied by the (1×2) and (2×1) superstructures during electric-current heating is determined by the anisotropy of the surface diffusion, whose direction is related to the orientation of the dimers in the superstructure domains of various types, and by the effective charge of the adatoms. The islands at the (001) surface of silicon which had two-dimensional sublimation islands $a/4$ in depth were found to be asymmetric. The island has the shape of an ellipse, whose major axis is perpendicular to the orientation of the dimers of the superstructure at the bottom of the island. The asymmetric shape of the two-dimensional islands (the ratio of the minor axis to the major axis is 0.7–0.8) suggests that the direction at the (001) surface of silicon is that of the preferential diffusion of adatoms, whose appearance is attributable to the presence of dimers in the superstructure domains. It should be pointed out that the anisotropy of the diffusion processes, according to Ruzaĭkin *et al.*,[9] occurs even on an unreconstructed (001) surface of silicon. The anisotropy of a reconstructed surface is linked with the formation of chains along the ⟨110⟩ plane of the adatoms of alkali metals at the (001) surface of silicon in the case of submonolayer cladding.[10,11] The effective charge of an adatom, according to Nesterenko and Snitko,[1] is given by

$$z_{\text{eff}} = e(z_0 - nc_n l_n + pc_p l_p),$$

where z_0 is the degree of ionization of the atom, $c_{n,p}$ and $l_{n,p}$ are respectively the scattering cross sections and the path lengths of electrons (n) and holes (p), and e is the electron charge.

Under these conditions, the mechanism for the pairwise convergence of monatomic steps can be described as follows. The presence of an effective adatom charge leads to an increase of the inverse flux of adatoms at the step of those terraces whose direction of dimerization is parallel to the step line. In the experimental situation shown in Fig. 2b, for example, the inverse adatom flux on the upper steps of the terraces with the (2×1) structure increases, causing these steps to slow down with respect to the lower steps of the terraces. In the case shown in Fig. 2c, the velocity of the lower steps of the terraces with the (2×1) structure decreases. A change in the relative velocities of monatomic steps thus causes a pairwise convergence of the steps, which changes the relative areas of the (2×1) and (1×2) superstructures.

It is pertinent to note that according to the data in Fig. 2, $z_{\text{eff}} < 0$. Our conclusion concerning the presence of an effective adatom charge is consistent with the previously obtained results which showed that the direction of the direct electric current which heats the crystal has an effect on the echeloning processes of monatomic steps at the clean (111) surface of silicon.[12]

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