Anomalous behavior of monatomic steps in $(1\times1)\rightleftarrows(7\times7)$ reconstruction at an atomically clean silicon (111) surface

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Analysis of the behavior of monatomic steps on the silicon (111) surface by means of ultrahigh-vacuum reflection electron microscopy reveals a redistribution of a significant number of the atoms during the reconstruction $(1\times1)\rightleftarrows(7\times7)$.

Recent progress in the field of scanning tunneling microscopy[1,2] has resulted in the determination of the coordinates of atoms in the unit cell of the (7×7) superstructure on an atomically clean silicon (111) surface. The mechanism for the reversible reconstruction from the (1×1) structure into the (7×7) superstructure has not been determined, however, because of difficulties confronting attempts to obtain information on the kinetics of this structural phase transition.

In this letter we report the use of a method of ultrahigh-vacuum reflection electron microscopy, developed previously,[3] for an *in situ* study of the superstructural reconstruction which occurs at an atomically clean silicon (111) surface. Depending on the preparation conditions,[4] the surface will contain the following microrelief elements: a system of equidistant monatomic steps; a system of echelons of monatomic steps consisting of accumulations of steps separated by nearly singular terraces; two-dimensional negative islands, which arise during sublimation on terraces with a width greater than twice the diffusion length of the adatoms at the given sublimation temperature; and two-dimensional growth islands, which form in the initial stages of the growth of the epitaxial silicon film from the molecular beam directly in the ultrahigh-vacuum reflection electron microscope.

In this study we observed a displacement of monatomic steps toward a higher terrace during the $(7\times7)\rightarrow(1\times1)$ reconstruction and toward a lower terrace during the opposite transition (Fig. 1), by an amount equal to 0.2–0.3 of the width of the given terrace. The direction of the displacement of the monatomic steps which bound two-dimensional negative islands or growth islands (Fig. 2, b and c) corresponds to the direction of the displacement of the equidistantly spaced steps (Fig. 2a).

For two-dimensional islands of small dimensions, the magnitude of the displacement can be sufficient for the complete disappearance of these islands. For steps in echelons, the magnitude of the displacement of the steps during the reconstruction is determined by the width of the lower terraces adjacent to the steps. This effect leads to a change in the distance between the steps in the echelons, in accordance with Fig. 2d.

The intensity of the specularly reflected electron beam, measured with an electron detector built into the electron microscope, increases during the $(1\times1)\rightarrow(7\times7)$ phase transition and decreases during the opposite transition, by about an order of magnitude.

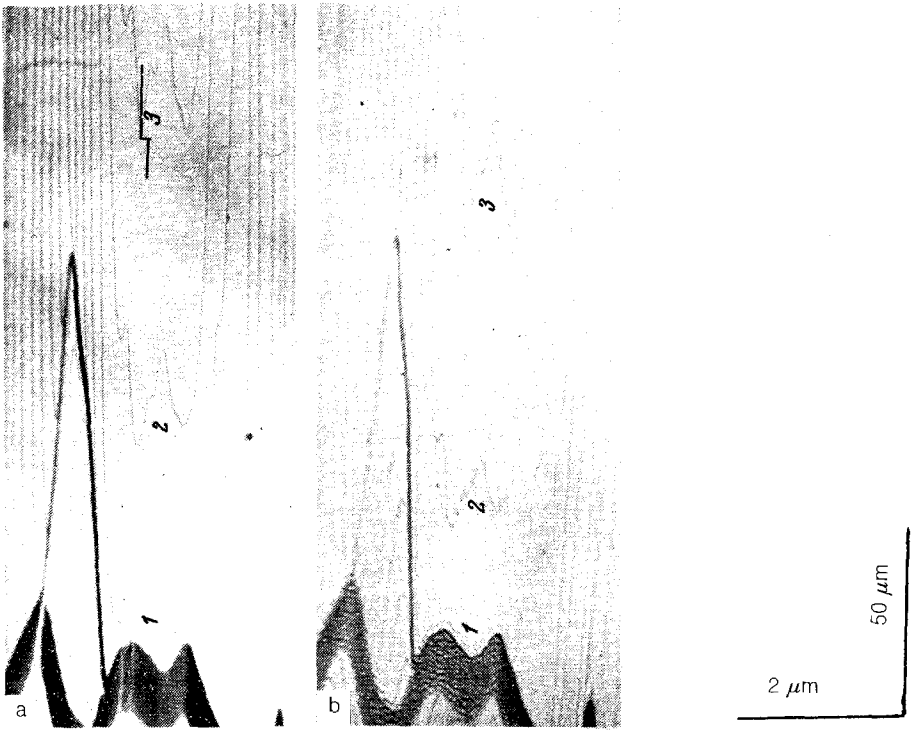

FIG. 1. a—Reflection electron micrograph of a silicon (111) surface with the (1×1) structure; b—after the $(1\times1)\rightarrow(7\times7)$ phase transition. The dark band is an echelon of closely spaced monatomic steps; the numbers label individual monatomic steps.

Since the displacement of a monatomic step remains constant during the $(1\times1)\rightarrow(7\times7)\rightarrow(1\times1)$ phase transitions, identical numbers of atoms migrate along the surface during the forward and inverse transitions. It also follows that we can ignore the desorption of atoms from the surface in this case. Working from the displacement of the monatomic steps, we can estimate the number of atoms which are

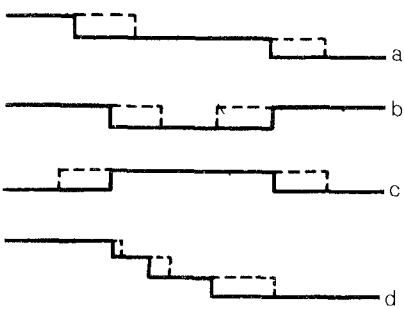

FIG. 2. a—*Model of the reversible displacement of monatomic steps along the surface of the silicon crystal during the* $(1\times1)\rightleftarrows(7\times7)$ transition in a system of uniformly spaced steps; b—during a change in the size of two-dimensional sublimation islands; c—during a change in the size of two-dimensional growth islands; d—in an echelon of steps. The solid line shows the position of the steps for the (1×1) structure, and the dashed line shows the position for the (7×7) structure.

absorbed by the steps during the $(1\times1)\rightarrow(7\times7)$ transition or which are generated by the steps during the inverse transition. The number of these atoms is 4×10^{14} cm^{-2}, or three or four orders of magnitude greater than the thermodynamic-equilibrium concentration of adatoms on the surface at the transition temperature, which is 10^{10}–10^{11} cm^{-2}, according to Ref. 5. The time required to generate this number of adatoms by a monatomic step during sublimation is more than 10^4 times the experimentally observed time of motion of the steps during the $(7\times7)\rightarrow(1\times1)$ transition.

According to the data of Refs. 1 and 2, the unit cell of the (7×7) superstructure contains 12 atoms in the first layer and a single vacancy in the second. If we assume that the (7×7) structure is formed from an atomically smooth (1×1) surface, then we would have to remove 80–90% of the atoms from the first completely filled layer and incorporate them in steps according to the model of Refs. 1 and 2. This number includes the atoms which form vacancies in the second layer. Exceptional cases are the 12 atoms of the first layer, which should simply undergo changes in position. Experimentally, one observes that only 0.2–0.3 of a monolayer drains off to steps during the $(1\times1)\rightarrow(7\times7)$ transition. It can therefore be suggested that the (1×1) surface is atomically rough, with a filling of 0.5. Since the lowering of the intensity of the specular reflection is usually explained on the basis of an increase in atomic roughness,[6] our experimental data on the behavior of the specularly reflected beam during the phase transition are also evidence in favor of the suggestion of a partial filling of the surface layer of the (1×1) structure.

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