Phase transition on stepped silicon surfaces

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(Submitted 7 September 1982)
Pis'ma Zh. Eksp. Teor. Fiz. **36**, No. 8, 290–292 (20 October 1982)

Phase transitions are discovered on clean silicon surfaces inclined away from (111) toward $[2\bar{1}\bar{1}]$ planes. At temperatures below 850 °C, systems of ordered steps with height equal to three interplanar distances d_{111}, which reform reversibly into steps with height equal to a single interplanar distance above 850 °C, form on such surfaces.

PACS numbers: 64.70.Kb, 68.20. + t

As shown previously,[1–3] reversible order-order and order-disorder phase transitions occur on clean germanium and silicon surfaces at certain temperatures, including on clean vicinal silicon surfaces inclined away from the (111) toward the $[\bar{2}11]$ planes.

The purpose of this paper is to report a reversible phase transition observed with the help of low-energy electron diffraction (LEED) on silicon surfaces inclined away from the (111) plane toward the $[2\bar{1}\bar{1}]$ plane.

It is well known[7] that systems of ordered atomic steps, i.e., steps with identical terrace height and width, form on clean vicinal (111) silicon surfaces. In LEED patterns from stepped surfaces, the diffraction reflections split into multiplets. The terrace width can be determined from the angular splitting of the reflections, while the height of a step can be determined with high accuracy by measuring the energy of electrons for which a definite reflection is observed in the form of a singlet.[5,6] Since the (111) plane has an odd-(third) order symmetry axis, two types of steps can form, depending on the direction of rotation of the surfaces of the plane around the directions $[01\bar{1}]$. In an ideal lattice (see Fig. 1), the atoms at the edges of the steps with the leading edge along $[\bar{2}11]$ have three nearest neighbors and a single cut bond, while atoms with leading edge along $[2\bar{1}\bar{1}]$ have two nearest neighbors and two cut bonds.

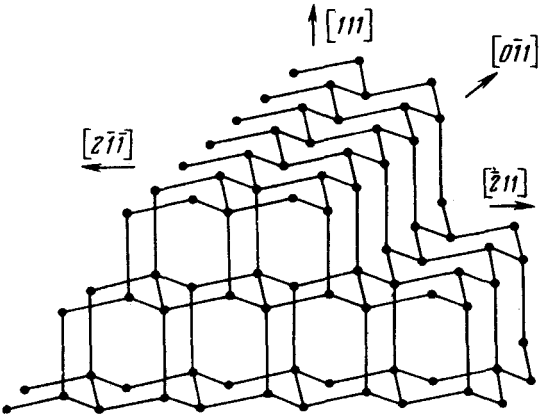

FIG. 1. Model of atomic steps on (111) surface of silicon in an ideal lattice.

It was reported previously[1-4] that reversible restructuring of steps with height equal to one interplanar spacing into steps with height equal to two interplanar spacings occurs on surfaces inclined away from the (111) plane to the $[\bar{2}11]$ plane. In our work, we investigated the surfaces inclined away from the (111) plane toward the $[2\bar{1}\bar{1}]$ plane. Steps with leading edge on $[2\bar{1}\bar{1}]$ were observed on silicon surfaces prepared by superhigh-vacuum cleavage.[7] These steps had a height equal to a single interplanar spacing and after annealing at a temperature above 600 °C, they coalesced. In our work, we investigated specimens inclined at angles from 3 to 11.50. The specimens were oriented with the help of an x-ray method. In order to avoid spoiling the layer on the surface, after grinding and polishing, the specimens were oxidized to a depth of about 1 μm. Before the chamber was placed in a vacuum, the oxide was removed from the surface of the specimens by dissolving in hydrofluoric acid vapor. Steps with height equal to a single interplanar spacing are already observed on surfaces prepared in this manner even before cleaning.[8] The specimen surfaces were cleaned by heating in a vacuum of $(1-2)\times 10^{-10}$ mm Hg. After heating at a temperature of 700 °C, LEED patterns corresponding to the Si(111)–7×7 structure were observed from all surfaces studied, even though they were not completely cleaned. This indicates that the steps coalesced and regions formed on the surfaces with (111) orientation with dimensions greater than the electron-coherence length, which is of the order of 100 Å. Diffraction patterns were again obtained from the stepped surface only after heating at a temperature of about 1.250 °C. Auger spectra did not show in this case the presence of impurities. After obtaining a clean surface using the method described above, we investigated the behavior of the LEED patterns at different specimen temperatures. The LEED pattern observed at specimen temperatures below 850 °C (see Fig. 2a) corresponds to surfaces containing ordered steps with (111) terraces and height equal to three interplanar distances d_{111}, which is indicated by the alternation of singlets as the electron energy varied, as well as the angular splitting of the reflections at a given angle of inclination of the (111) surface. For small angles of inclination of the surface, the terrace dimensions are comparable to the electron-coherence length and the LEED patterns from such surfaces exhibit reflections of orders that are multiples of 1/7 from the Si (111)-7×7 structure on terraces. At the same time, because of the decrease in the angular splitting of reflections, it is difficult to determine the step parameters.[4] At a

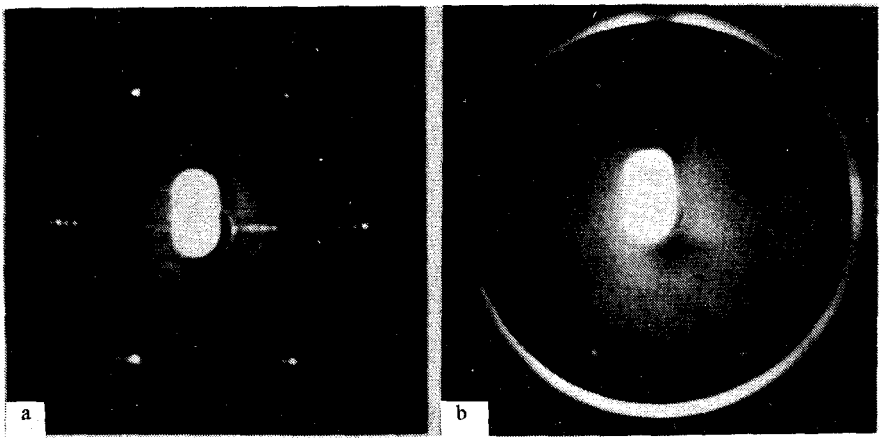

FIG. 2. LEED patterns from (755) Si surface. The angle with the (111) plane is 9.45°. The electron energy is 47 eV. (a) 740 °C; (b) 870 °C.

temperature of about 850 °C, a reversible restructuring of the surface occurs. The LEED patterns obtained in this manner (Fig. 2b) correspond to diffraction from equidistance steps with (111) terraces, but with height equal to a single interplanar distance and a three times narrower terrace. As the specimen temperature decreases, two reflections that disappeared with heating appear again between the reflection on the pattern in Fig. 2b, i.e., the previous system of steps is formed once again. The reflections present in the pattern in Fig. 2b remain at all specimen temperatures.

The time for one system of steps to restructure into another is comparable to the time for establishing the specimen temperature with a change in the heating current. For this reason, it was not possible to study the kinetics of the process by measuring the dependence of the reflection intensities as a function of time for different temperatures, as done in Refs. 9 and 10. There is no appreciable hysteresis in the phase transitions. We note that hysteresis was not observed in transitions Si (111)-7×7⇌Si (111)-1×1,[11] which are first-order transitions.[12]

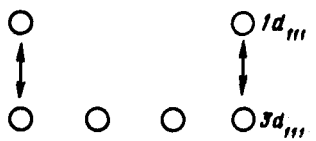

FIG. 3. Diagram showing the change in the multiplet accompanying the phase transition.

We thank A. I. Nikiforov, who participated in the experiments at the first stage of the work.

[1]B. Z. Ol'shanetskiĭ, S. M. Repinskiĭ, and A. A. Shklayev, Pis'ma Zh. Eksp. Teor. Fiz. **25**, 195 (1977) [JETP Lett. **25**, 195 (1977)].
[2]B. Z. Ol'shanetskiĭ, in: Problems in the Physics of Semiconductors. Proceedings of the IXth Winter School on the Physics of Semiconductors, A. F. Ioffe Physicotechnical Institute, Academy of Sciences of the USSR, Leningrad, 1979, p. 140.
[3]B. Z. Ol'shanetskiĭ, Stud. Surf. Sci. Catal. **9**, 214 (1982).

[4]B. Z. Ol'shanetskiĭ and A. A. Shklyev, Surface Sci. **82**, 445 (1979).
[5]M. Henzler, Surface Sci. **19**, 159 (1970).
[6]B. Z. Ol'shanetskiĭ, A. I. Nikiforov, and V. I. Mashanov, Fiz. Tverd. Tela **23**, 3136 (1981) [Sov. Phys. Solid State **23**, 1825 (1981)].
[7]M. Henzler, Surface Sci. **36**, 109 (1982).
[8]B. Z. Ol'shanetskiĭ and A. V. Rzhanov, Pis'ma Zh. Eksp. Teor. Fiz. **32**, 337 (1981) [JETP Lett. **32**, 313 (1981)].
[9]B. Z. Ol'shanetskiĭ, S. M. Repinskiĭ, and A. A. Shklyaev, Pis'ma Zh. Eksp. Teor. Fiz. **27**, 403 (1978) [JETP Lett. **27**, 378 (1978)].
[10]B. Z. Ol'shanetskiĭ and A. A. Shklyaev, Zh. Eksp. Teor. Fiz. **81**, 361 (1980) [Sov. Phys. JETP **54**, 194 (1981).
[11]P. A. Bennett and M. W. Webb, Surface Sci. **81**, 361 (1981).
[12]N. Osakabe, Y. Tanishiro, K. Yagi, and G. Honjo, Surface Sci. **109**, 353 (1981).

Translated by M. E. Alferieff
Edited by S. J. Amoretty