Possibility of investigating surface self-diffusion of silicon by the slow-electron diffraction method

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(Submitted 1 February 1978)
Pis'ma Zh. Eksp. Teor. Fiz. **27**, No. 7, 403–405 (5 April 1978)

The possibility is demonstrated of investigating surface self-diffusion by determining the kinetics of surface restructuring in phase transitions of the order–order type on clean semiconductor surfaces.

PACS numbers: 66.30.Fq, 68.90.+q

Surface self-diffusion of atoms determines the character of many processes that occur on the surface of a solid. However, the information contained in the literature on the parameters of the surface self-diffusion on semiconductors, is highly insufficient. This is due to the complexity of the surface self-diffusion processes and to the limited possibilities of investigating processes under clean conditions. Since the use of direct observation methods of surface self-diffusion (with the aid of an ion field-emission microscope) is difficult in the case of semiconductors, great importance for the study of surface self-diffusion is attached to experiments connected with mass transport on single-crystal surfaces, due to minimization of the surface free energy.[1] An example of such research is the work performed in an electron field-emission projector.[2–4]

As will be shown below, surface diffusion of germanium and silicon can be investigated by studying the kinetics of the restructuring of pure surface under reversible phase transitions of the order-order type, a number of manifestations of which have been described previously.[5–8] On pure silicon surfaces oriented in the [011] zone at small angles to the (100) plane there are ordered steps, the heights of which are equal to two interplanar distances and are stable over the entire temperature range in which it was possible to observe the slow-electron diffraction (SED) processes–up to 1050 °C. On surfaces close to (110) in orientation, at the same temperature, facet planes of the type (47 35 7) were observed, making an angle 10°42′ with the (110) plane. The surfaces oriented in the $[\bar{1}10]$ zone at small angles to the (111) plane can contain steps with fronts along $[2\bar{1}\bar{1}]$ or with fronts along $[\bar{2}11]$, depending on the direction of rotation of the surface. In the former case the steps have a height close to one interplanar distance. These steps vanish when the sample is annealed in vacuum.

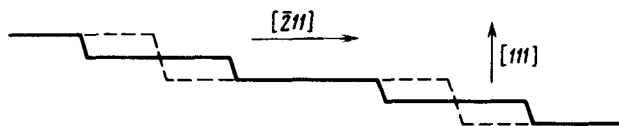

FIG. 1. Scheme of restructuring of steps with front along $[\bar{2}11]$ on the (111) surface of silicon. The solid line denotes steps with height of one interplanar distance, the dashed line–with height of two interplanar distances.

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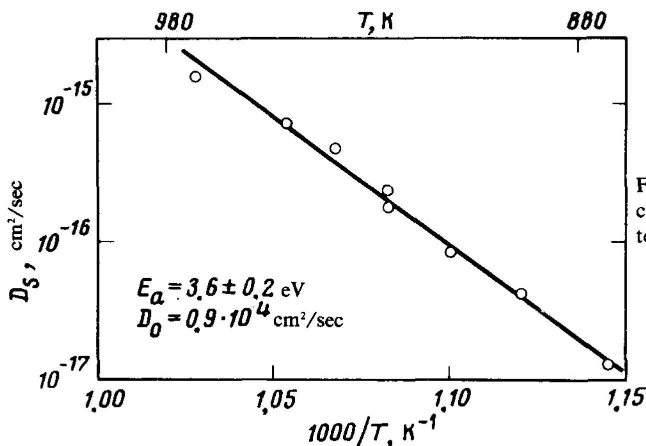

FIG. 2. Dependence of the coefficient of diffuse mass transfer on the temperature.

Steps with front along [$\bar{2}$11] have at a temperature below 800 °C a height equal to two interplanar distances. At 800 °C a reversible restructuring of these steps into steps with height of one interplanar distance takes place (Fig. 1). Analogous structural transitions on the surface of germanium are observed near 500 °C.[8] The formation of steps having a height of two interplanar distances is accompanied by the appearance of additional reflections on the SED patterns.

The restructuring of the surface is connected with transport of matter, and its time depends on the temperature. We shall assume that the process of restructuring of the surface consists of a detachment of the atom from the break of the step and subsequent diffusion of the atom over a terrace with orientation (111) towards the alignment point. Then the expression describing the process of surface restructuring can be written in the form[1]

$$D_s = D_0 \exp(-E_a/kT) = \frac{\langle r^2 \rangle}{2t},$$

where D_s is the coefficient of the diffuse mass transport, E_a is the activation energy, k is Boltzmann's constant, T is the absolute temperature, D_0 is the pre-exponential factor, $\langle r^2 \rangle$ is the mean-squared displacement of the atom by diffusion, and t is the time of detachment and diffusion of the atom over the corresponding distance. By investigating the dependence of the time of restructuring of the surface on the temperature with the aid of the intensities of the additional reflections, we can obtain the value of the activation energy of the restructuring process. The measurements were performed on silicon samples whose surface was rotated 8° relative to the (110) plane in the [$\bar{1}$10] zone. The obtained activation energy for the restructuring process of the steps with height of one interplanar distance into steps with height of two interplanar distances is 3.6±0.2 eV. To estimate the pre-exponential factor, $\langle r^2 \rangle$ was chosen equal to the square of the width of the terrace of steps of height of one interplanar distance, while t was chosen equal to the restructuring time as measured in the experiment. The value of the pre-exponential factor was found to be 9×10^3 cm²/sec (Fig. 2). The obtained

value of the activation energy is approximately 3/4 of the activation energy of the self-diffusion of the silicon in the volume.[9,10]

As seen from[5-8], the phase transitions connected with the transport of matter are a sufficiently common property of the surfaces of the single-component semiconductors. Their investigation offers new possibilities of the study of the surface self-diffusion of the semiconductors. Advantages of the described method are the possibilities of investigating diffusion on a definite face under conditions of ultrahigh maximum, multiple reproduction of the initial surface, and variation of the distance over which the matter is transported by the change of the surface orientation.

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