Effect of a structural change in the silicon surface on the diffusion of potassium and sodium on it

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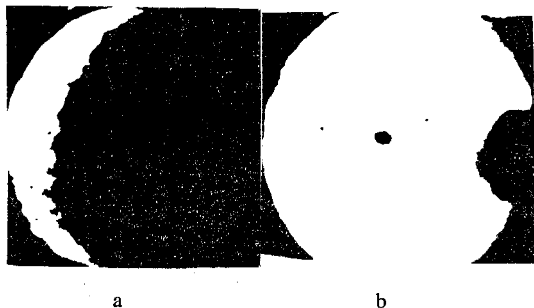
The diffusion of potassium and sodium on a silicon surface, cleaned by field evaporation and changed by high-temperature ($T \geq 700$ K) heating, was studied by the method of field-emission spectroscopy. After the surface was changed, the diffusion coefficient increased by more than three orders of magnitude.

The diffusion of metal atoms in semiconductors has been studied primarily in extended samples with a "real" surface that generally contains many structural defects and impurities. In the present experiments we studied the surface diffusion of alkali metal atoms in silicon by the method of field-emission microscopy. The use of this method produces a clean surface with uniform properties such as those obtained in Ref. 1.

The field-emission cathodes were fabricated from a highly pure silicon crystal, whose concentration of the alkali impurities, determined by neutron-activation analysis, was lower than 10^{12} cm^{-3}. The point of the field-emission cathode was made atomically pure by field evaporation of layers from it first in a hydrogen atmosphere and then in a vacuum, after the appropriate heat treatment, as in Ref. 2. It was shown in Ref. 2 by the method of field-ion microscopy that a surface prepared in this manner does not have any steps and is smooth.

The sodium and potassium, purified by repeated distillation in a vacuum, entered the lateral surface of the point from a molecular beam at a residual gas pressure of $p = 10^{-10}$ Torr in the experimental apparatus. A piezoquartz microbalance was used to estimate the flux of atoms.

The diffusion occurred in the absence of an electric field. A voltage was applied to



a b

FIG. 1. (a) Boundary of the adsorbate film deposited on the tip of a structurally unaltered point. (b) Same boundary after 4 minutes.

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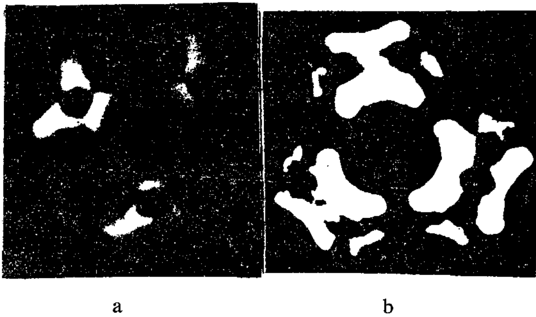

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FIG. 2. (a) Field-emission image of a silicon point whose surface has been structurally altered by heating the sample to 1500 K; (b) field-emission image of the same point 5 seconds after two monolayers of potassium were deposited on the lateral surface of the point.

the point only for the time required to photograph its field-emission image. The surface-diffusion coefficient was estimated from the time required for the boundary of the adsorbate film, visible under a field-electron microscope (Figs. 1a and 1b), to move a certain distance, determined from measurements of the dimension of the point in a scanning electron microscope. With a radius of curvature of the point of 1 μm, the advancement of the boundary at room temperature in a time of 4 minutes is estimated from a comparison of Figs. 1a and 1b to be 1.5 μm. This gives the value $D \simeq 10^{-10}$ cm^2/s.

Heating the field-emission cathode, which was first cleaned by field evaporation, at $T \geq 700$ K leads to a structural change of its tip and to the appearance of a distinct single-crystalline faceting (Fig. 2a). On a surface changed in this manner, the propagation of adsorbates across the tip of the point occurs so rapidly that the entire emitting surface of the field-emission cathode is covered by the adsorbate in several seconds required to switch off the sources of alkali atoms and to switch on the field-emission field. The movement of the boundary of the adsorbed film could not be recorded, even after cooling the sample with liquid nitrogen. Figure 2b shows the field-emission image of the point 5 seconds after two monolayers of potassium were deposited on its lateral surface. It is evident that by this time the diffusion process has completely terminated. An estimate shows that after rearrangement of the surface, the diffusion coefficient increases by more than three orders of magnitude.

This strikingly sharp increase of the diffusion coefficient of alkali-metal atoms, after changing the silicon surface, shows that the diffusion-activation energy decreases appreciably.

The silicon surface obtained after evaporation in an electric field is characterized, as we know, by a density of surface electronic states (SES) of about 10^{15} cm^{-2}. The electrons belonging to the alkali atoms that reach the surface can be captured into these states, thus forming a strong ionic adsorption bond between the atoms and the substrate.

After changing the surface of the sample by heating, the density of SES decreases by several orders of magnitude. For this reason, these states no longer play a key role

in the adsorption. Furthermore, an alteration of the surface changes its atomic structure. Thus, for example, the (111) surface of silicon acquires a 7×7 structure. These factors, taken collectively change the adsorption bond and the potential relief of the surface, causing the diffusion activation energy and the diffusion coefficient also to change.

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