# Determination of the migration energy of vacancies and of intrinsic interstitial atoms in silicon in the temperature interval 400–600°K

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(Submitted May 5, 1976)
Pis'ma Zh. Eksp. Teor. Fiz. **23**, No. 12,688–691 (20 June 1976)

We present experimental data on the direct determination of the migration energy and the diffusion coefficient of point defects, identified as vacancies and intrinsic interstitial atoms, in silicon.

PACS numbers: 61.70.Fz, 66.30.Kv

There is still no meeting of minds in the literature concerning the parameters of the migration of the simplest defect in germanium and silicon. For example, indirect experimental estimates and theoretical calculations of the vacancy migration energy ($E_m$) in silicon lie in the wide range from 0.18 to 1.09 eV.[1]

We describe here an experiment aimed at a direct determination of $E_m$. It is based on the high sensitivity of photostimulated electron emission (PSEE) to small deviations of the concentration of point defects from equilibrium,[2] and on a specially developed procedure, according to which the point defects are produced by irradiation of one surface of the sample, while the PSEE is measured on the opposite surface.[3] In this experimental geometry one monitors in the experiment the length of the diffusion path (the thickness of the sample) and the time required by the defects to negotiate it. The kinetics of PSEE is determined in this case by the time dependence of the flux of point defects reaching the emitting surface.[4]

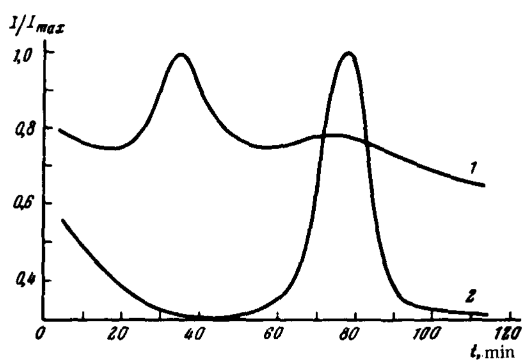


Fig. 1. Kinetics of PSEE intensity after bombardment: 1) silicon ($L = 330\ \mu$; $T = 170\ °C$), 2) aluminum ($L = 80\ \mu$; $T = 450\ °C$).

  

Nonequilibrium point defects were produced in the investigated single-crystal silicon samples by bombardment with an ion-plasma beam (ion energy ~3 keV) produced by the procedure of [5].

The PSEE was registered in a vacuum of $\sim 10^{-5}$ Torr with a secondary electron multiplier, the sample being illuminated with light from a mercury lamp through a light filter.

Figure 1 shows a typical time dependence of the PSEE intensity after irradiation. It is seen from Fig. 1 that the PSEE after the bombardment decreases monotonically to the level of the "background" and maxima then appear on the kinetic curves. The positions of the maxima on the PSEE kinetic curves are determined by the sample thickness ($L$) and by the temperature ($T$): the maxima shift into the region of shorter times with decreasing $L$ or with increasing $T$, and the opposite is observed with increasing $L$ and decreasing $T$. This effect points to a connection between the maxima of the PSEE and the migration of the point defects through the sample, since the flux at the point defects near the emitting surface also has a maximum with respect to time.

We have performed special experiments showing that extraneous effects that take place in ion-plasma bombardment (local heating of the sample, acoustic excitation, etc.) produce only a monotonically damped PSEE. The influence of the extraneous effects on the PSEE was verified also by substituting aluminum for the silicon. The character of the PSEE kinetics of bombarded aluminum (Fig. 1) was similar to that of Si, and its temperature dependence indicates that the maximum of the kinetics is connected with diffusion of divacancies in the aluminum. [4]

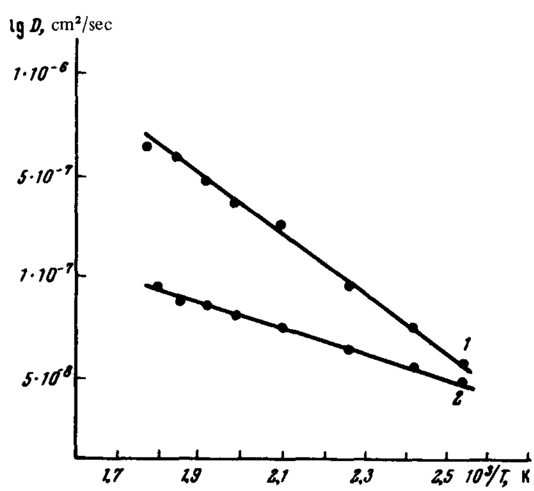


FIG. 2. Temperature dependence of the diffusion coefficient of vacancies (1) and of intrinsic interstitial atoms (2) in silicon.

The type of defects and their diffusion parameters were determined with the aid of the diffusion equation

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - ac, \qquad (1)$$

where $c$ is the defect concentration.

From the solution of (1) it is easy to obtain an expression for the point-defect flux at the emitting surface, the time of arrival of the maximum of which ($t_M$) is equal to $t_M \approx L^2/2\sqrt{\alpha D}$ in the case of intense capture ($\alpha \gg L^2/D$) and to $t_M \approx L^2/6D$ [2] at $\alpha \approx 0$. Knowing $L$ and $t_M$ we can determine the diffusion coefficient of the defects. It should be noted that the presence of point-defect capture influences only the magnitude of the pre-exponential factor in the diffusion coefficient, but does not influence the migration energy, which is determined from the temperature dependence of $D$.

We have carried out the measurements in the temperature interval 100—350°C. Figure 2 shows the temperature dependence of the diffusion coefficient calculated from [2] without allowance for capture. The pre-exponential factor in the Arrhenius equation turned out to be $D_{01} = (2.2 \pm 0.1) \cdot 10^{-4}$ cm$^2\cdot$sec$^{-1}$ for the former type of defect and $D_{02} = (1.1 \pm 0.1) \cdot 10^{6}$ cm$^2\cdot$sec$^{-1}$ for the latter. The corresponding migration energies are $E_{m1} = 0.30 \pm 0.04$ eV and $E_{m2} = 0.12 \pm 0.04$ eV.

The numerical values of the diffusion parameters of the point defects allow us to assume that defects of the first type are vacancies ($D_{01}$) and of the second type ($D_{02}$) are intrinsic interstitial atoms. Our values of the migration energies agree well with the estimates of [6].


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