Temperature-Dependent Defect Production in Bombardment of Semiconductors*

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A model is proposed to explain the observed dependence of the defect production rate on temperature when semiconductors are bombarded with electrons of sufficient energy to produce vacancy-interstitial pairs. The decreased defect density observed after low-temperature bombardment may be due to the production of a metastable vacancy-interstitial pair which may either anneal or form the defect usually observed. A temperature dependence in the production rate arises if these two competing processes have different activation energies.

IN a recent experiment it was noted that the rate of production of a certain defect by high-energy electrons in silicon is strongly dependent on the temperature at which the bombardments are made.[1] More specifically, it was found that the energy level located 0.16 ev below the conduction band is produced in lower density the lower the temperature of the specimen during bombardment. Figure 1 shows data for one sample bombarded at 0.7 Mev. The defect introduction rates were obtained from small changes in conductivity all measured at the same temperature of 200°K. They are plotted at the bombardment temperature. Two sets of points are shown; the triangles refer to introduction rates obtained on going from the bombardment temperature immediately to the measuring temperature, the circles to introduction rates after a 5-minute anneal at 333°K. The measuring temperature was chosen so that the defect level was at least 95% filled with electrons.

Similar observations have recently been made in a number of other experiments. In the study of spin resonance it was found that the density of a defect tentatively identified with the 0.16-ev level was reduced by a large factor if the specimen is bombarded at liquid nitrogen temperature.[2] This effect, in terms of carrier removal but of lesser magnitude, was also noted by Hill[3] in an extensive series of measurements on electron-bombarded silicon. In germanium a similar effect has been observed by Brown in experiments extending down to 20°K.[4] He also found that the effect was more pronounced the lower the bombarding energy.

Results of this nature may be understood in terms of the following model of the damage process. We consider damage produced by electrons having sufficient energy to displace lattice atoms to nearby interstitial positions as a result of an electron-nuclear encounter. The displacement process occurs in a time short compared to the time required for motion of the neighboring atoms, so that the struck atom moves through an undistorted lattice.[5] Subsequently the lattice around the vacancy just produced will relax. We now enquire as to the nature of the potential energy of the displaced atoms in their local equilibrium positions. It is clear that at some large distance from the defect the potential minima will all be identical. In the immediate vicinity of the vacancy the inward motion of the atoms surrounding it can create a more favorable position for the interstitial, Fig. 2. This inward motion may also result in a barrier which makes the last few jumps of the interstitial toward the vacancy more difficult. This is similar to a proposal made by Fletcher and Brown.[6] One additional feature of the potential energy diagram proposed here is that the first interstitial position, corresponding to a vacancy-interstitial (V-I) pair in ⟨111⟩ orientation, is highly unstable. Interstitials which

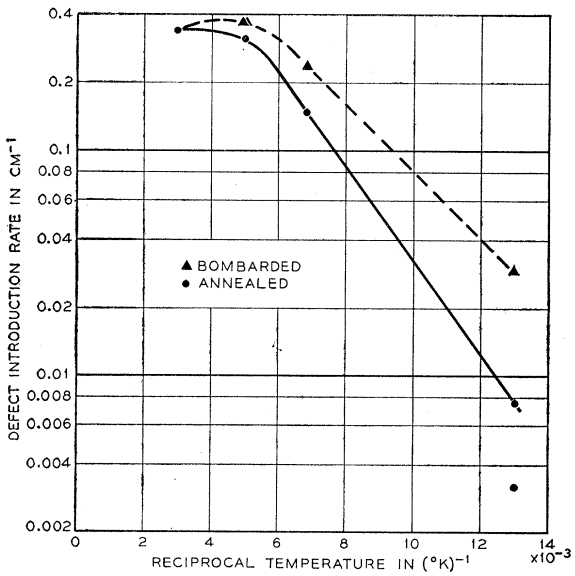

FIG. 1. Rate of introduction of damage in silicon by 0.7-Mev electrons as a function of sample temperature during bombardment. The introduction rate is measured per unit of bombarding flux and represents the number of defects formed per cubic centimeter for each electron per square centimeter incident on the sample.

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[1] G. K. Wertheim, Phys. Rev. **110**, 1272 (1958).
[2] G. Bemski (private communication).
[3] D. E. Hill, thesis, Purdue University, 1959 (unpublished).
[4] W. L. Brown (private communication).
[5] W. Kohn (unpublished).
[6] R. C. Fletcher and W. L. Brown, Phys. Rev. **92**, 585 (1953).

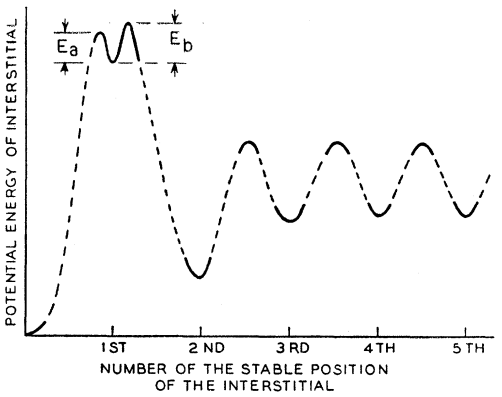

FIG. 2. A proposed potential energy diagram for an interstitial atom in the vicinity of a vacancy.

populate this position may either fall back into the vacancy annihilating the damage, or they may jump into the second V-I configuration creating a relatively stable defect pair. Interstitials which are displaced to the second V-I position will remain there; and those displaced to the third or other positions may be free to move at room temperature and will either diffuse away or else form stable pairs in the second V-I configuration. The net result is the formation of three distinct defects, a close-spaced pair in second V-I position and two essentially isolated defects.†

The two processes which compete in the destruction of the ⟨111⟩ pair will have thermal activation energies corresponding to the small barriers E_a and E_b. If these two barriers are not equal, the fraction of atoms going into the second V-I configuration rather than falling back into the vacancy will depend on temperature. In particular, if the barrier E_b is greater than the barrier E_a, the number of stable pairs formed by bombardment at low temperature will be smaller than that formed at high temperature. An estimate of the barrier heights required can be obtained in the following way: At 77°K the destruction of the ⟨111⟩ pairs is complete in a time short compared to that required to make a measurement after bombardment, i.e., of the order of minutes. Since the jump-time τ is given by

$$\tau=\nu^{-1}\exp(E/kT), \tag{1}$$

where ν, the lattice frequency, may be taken to be 10^{13} sec^{-1}, we find that the barrier height must be no greater than 0.3 ev. On the other hand, the fraction of ⟨111⟩ pairs which jump into the second V-I configuration is given by

$$f=1\Big/\left[1+\gamma\exp\left(\frac{E_b-E_a}{kT}\right)\right], \tag{2}$$

where γ is the ratio of the statistical weights of the jump which annihilates the defect to that which forms the stable pair. This function has the shape of the curve shown in Fig. 1, and the slope of the curve at low temperature gives the difference in barrier heights which turns out to be 0.04 ev.

The small size of the barrier obtained above raises the question why the struck atom, which retains energies of a few electron volts after leaving its equilibrium position, remains in this shallow potential minimum. This difficulty does not arise in actual fact, however, since the displacement process takes place in an undistorted lattice as indicated above. The relaxation of the lattice into the configuration which gives rise to the barrier and shallow minimum takes place after the struck atom has lost its kinetic energy in collisions with its neighboring atoms.

This model is in accord with a number of other observations. For example, the defect production rate at 0.7 Mev is much smaller than the displacement probability computed from a threshold energy of 13 ev.[7] In terms of the present model, this means that many of the defects produced annihilate. Secondly, the observation of a number of distinct energy levels in electron-bombarded silicon[1,3] follows from the production of a number of distinct damage configurations by the processes described above. Finally, the dependence on bombarding energy observed by Brown[4] agrees with this model, since low-energy collisions preferentially populate the near ⟨111⟩ sites.

† *Note added in proof.*—The essential arguments remain unchanged if the potential minimum at the second V-I position is not sufficiently deep to stabilize the close-spaced V-I pair configuration. In this case the jump of the interstitial from the metastable position either annihilates the defect as before, or liberates the interstitial from the vacancy allowing either or both of them to diffuse to other trapping sites.

[7] J. J. Loferski and P. Rappaport, Phys. Rev. **111**, 432 (1958).