Configurationally bistable defects in silicon

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Defects having two different structural configurations in an isoelectronic state have been discovered in silicon. The properties of the defects and the parameters of the configurational transition have been determined.

Among the most interesting defects in semiconductors today are centers exhibiting a strong electron-lattice interaction, e.g., U-centers, which are defects with a negative correlation energy.[1,2]

In the present letter we report a study of defects in silicon which undergo configurational transitions while remaining in the same charge state. The defects are induced in n-type silicon ($n_0 = 10^{14}$ cm^{-3}) by γ-ray bombardment with a ^{60}Co source. The parameters of the defects are determined by the method of time-varying capacitive spectroscopy, which can yield the concentrations of defects in various energy states and the energy of the thermal activation of carrier capture and emission. In our case, depending on the experimental conditions, we detect two signals, corresponding to energies $E_A = 0.12$ eV and/or $E_B = 0.18$–0.19 eV for thermal activation of the emission of electrons into the conduction band. In the case in which the centers are filled by short pulses of electrons ($t \leqslant 10^{-5}$ s), we detect signal A and not signal B. As the length of the filling pulses is increased, the amplitude of signal A falls off, while that of signal B increases (Fig. 1). When the pulse repetition period is much longer than the time constant for thermal emission of electrons for signal B, we find that the amplitudes of signals A and B satisfy the relation $\Delta C_A(t) + \Delta C_B(t) = \text{const}$.

We can thus conclude that the energies for the thermal activation of emission, E_A and E_B, correspond not to two different defects but the same defect in two states. For durations of the filling of centers with electrons which are much shorter than the scale time for transitions of the electrons from state A to state B, we find only state A

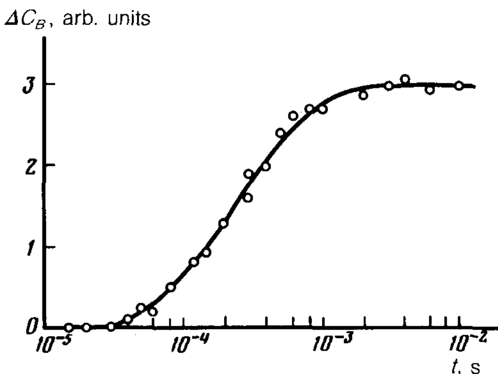

FIG. 1. Concentration of the B1 defect in state B versus the length of the filling pulses.

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experimentally, with an energy E_A for the thermal activation of emission. As the length of the filling pulses is increased, the defects undergo transitions to state B after capturing an electron, thereby reducing the amplitude of the signal of thermal emission characterizing state A. At the same time, the relative number of states B increases, and at $t \gg \tau_t$ (τ_t is the scale time for the configurational transition $A \rightarrow B$) we find only defects with the energy E_B for thermal activation of emission. The concentration of centers in state B (at the transition $A \rightarrow B$) is described by $N_B(t) = N_0\left[1 - \exp\left(\frac{-t}{\tau_t}\right)\right]$, where N_0 is the concentration of centers which have captured an electron at the initial time.

The transition time in turn depends on the temperature and is described well by the model of a first-order reaction, $\tau_t = \tau_0 \exp\left(\frac{-E_T}{kT}\right)$, where $E_T = 0.15$ eV is the activation energy for the transition $A \rightarrow B$ and $\tau_0^{-1} = 2.8 \times 10^{12}$ s^{-1} is a frequency factor.

The observed transitions can be explained by the two alternative configurational-coordinate diagrams in Fig. 2, a and b. Curve A^n (B^n), which is common to the two states,[3] corresponds to the unfilled state of a center in the presence of a free electron-hole pair. Depending on the sample temperature and the time over which the centers are filled with electrons, the defects undergo transitions to the state described by either curve A^{n-1} or B^{n-1}, which are characterized by a new equilibrium value of the generalized coordinate, Q_A or Q_B, respectively. At low temperatures and for short filling pulses ($t \leqslant 10^{-5}$ s), the capture of an electron puts the system in the state A^{n-1} with the equilibrium value $Q = Q_A$. The energy E_A corresponds to a thermally activated transition from state A^{n-1} to A^n. The transition of the system to state B^{n-1} is limited by the barrier E_T. As the temperature and the length of the filling pulses are increased, the probability for overcoming the barrier E_T increases, and the defects go

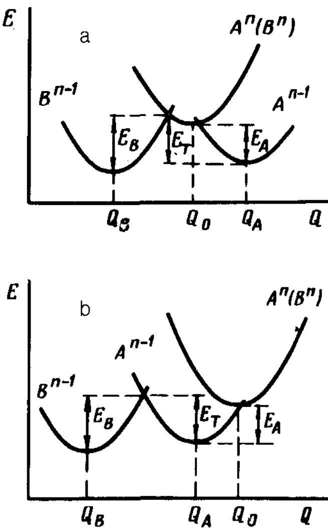

FIG. 2. Configurational-coordinate diagrams for the B1 defect (E is the total energy, and Q is the generalized coordinate).

into state B^{n-1}, with the equilibrium value Q_B of the generalized coordinate. The transition of the system from the state B^{n-1} to B^n (A^n) is determined by the thermal-emission energy E_B. For the diagram in Fig. 2a, this energy is $E_B = 0.18$ eV, while for that in Fig. 2b it is $E_B = 0.19$ eV. Since the state B^{n-1} at the equilibrium value $Q = Q_B$ has a total energy smaller than that of the state A^{n-1} ($Q = Q_A$), configuration B is stable, while configuration A is metastable. The data currently available do not point to either of these configuration diagrams as preferable.

The formation of the centers (B1) described above was observed in silicon with a low oxygen concentration ($\leqslant 10^{16}$ cm^{-3}). In these samples we detect, in addition to the B1 defects, centers with an energy of 0.18 eV for the thermal activation of emission, and for which the transition processes discussed above are not observed. We did not observe transitions of defects with the same thermal-activation energy for emission in samples with a high oxygen concentration ($\approx 10^{18}$ cm^{-3}). These facts are evidence that the B1 defect cannot be linked with an A center in silicon. This assertion is supported by data on the thermal stability of the B1 defect, which is annealed out in the interval 200–250 °C, while we observe the annealing out of the A center at $T < 300$ °C in the same samples.

In summary, the model of a bistable configuration of a defect explains the observed transformation of the energy spectrum for thermal emission of electrons and the change in the concentration of B1 centers in different states in a study of carrier capture and emission. We have determined the energies for the thermal emission of electrons from states A and B into the conduction band, $E_A = 0.12$ and $E_B = 0.18$–0.19 eV, respectively, and the barrier separating these states, $E_T = 0.15$ eV. The results show that the B1 defect is not a center containing oxygen.

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