Configurational reorganization of bistable defects in semiconductors

N. V. Kuznetsov and V. N. Filatov
Scientific-Research Institute of Nuclear Physics, M. V. Lomonosov Moscow State University

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The accumulation of the metastable state and the ground state of a bound electron in two different configurations of a bistable defect has been analyzed. The results are compared with experiment.

Time-dependent capacitive spectroscopy has revealed defects in semiconductors which have two or more configurational states of a bound electron.[1–4] In particular, Kuchinskiĭ *et al.*[64] observed a bistable defect in γ-bombarded n-type zone-refined silicon with metastable and ground states characterized by thermal-ionization energies $E_t = 0.12$ eV and $E_t = 0.18$–0.19 eV, respectively. Kuchinskiĭ *et al.* suggested two

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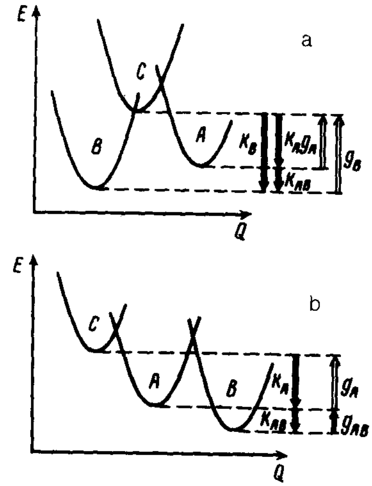

FIG. 1. Configuration diagrams of a bistable defect.

possible configurations of this defect, without giving preference to either. In the present letter we show that the question of the configuration of a bistable defect can be resolved by studying how the concentration of the ground state of a defect varies with the time over which it is filled by electrons. We will compare theoretical and experimental results for proton-bombarded silicon.

Figure 1, a and b, shows the two possible configuration diagrams of a three-level system of a bistable defect, according to Kuchinskiĭ *et al.*[4] Shown here are the electronic transitions which result in the transition of the defect from the state of a free electron (C) to a metastable state (A) or the ground state (B) of a bound electron, and vice versa, during charge exchange. On the basis of the relative positions of the various states of the defect along the configuration coordinate Q it can be asserted that for the first diagram (Fig. 1a) the transitions $C \to A$, $C \to B$, and $A \to B$ occur, with probabilities characterized by the coefficients k_A, k_B, and k_{AB}, respectively. Because of the high energy barrier for the $A \to B$ transition, the conditions k_A, $k_B > k_{AB}$, should hold. For the second diagram (Fig. 1b), the $C \to B$ transitions are improbable and can be ignored, while the relation between the coefficients k_A and k_{AB} is unknown.

In the method of time-varying capacitive spectroscopy of semiconductors, one measures the concentrations of the states of a bound electron, $N_A(t)$ and $N_B(t)$, which accumulate during a filling pulse t, in the stage of the thermal ionization of the electrons. The coefficients for the thermal ionization of the electrons, $g \sim \exp(-E_t/kT)$, or the thermal-ionization energy E_t are characteristics of the states which become freed of electrons.

Let us examine in detail the changes in the states of a bistable defect during the action of the filling pulse. This process can be described by a phenomenological theory of electronic transitions, according to which the following system of kinetic equations holds for the concentrations of free electrons, $N_C(t)$, and of bound electrons:

$$\frac{dN_C}{dt} = -k_A N_C \{-k_B N_C\}; \quad \frac{dN_A}{dt} = k_A N_C - k_{AB} N_A; \quad \frac{dN_B}{dt} = k_{AB} N_A \{+k_B N_C\}, \tag{1}$$

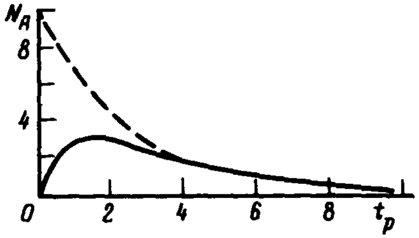

FIG. 2. Concentration of a metastable state versus the duration of the filling pulse.

The braces (curly brackets) contain terms which must be eliminated if the transitions that occur are those in Fig. 1b.

A solution of equations (1) under the conditions $N_C(0) = N$, where the right side is the total concentration of defects, and $N_A(0) = N_B(0) = 0$, is[1)]

$$N_A(t)/N = \frac{k_A}{k_1 - k_{AB}} [\exp(-k_{AB}t) - \exp(-k_1 t)]; \tag{2}$$

$$N_B(t)/N = \frac{k_A}{k_1 - k_{AB}} [1 - \exp(-k_{AB}t)] + \frac{k_2}{k_1 - k_{AB}} [1 - \exp(-k_1 t)], \tag{3}$$

where we have $k_1 = k_A + k_B$ and $k_2 = k_B - k_{AB}$ for the first scheme of electronic transitions (Fig. 1a) and $k_1 = k_A$, $k_2 = -k_{AB}$ for the second scheme (Fig. 1b). We are assuming $k_1 \neq k_{AB}$.

It can be seen from expression (2) that the curve of the concentration of the metastable state, $N_A(t)$, versus the time over which the filling pulse operates, t, has the same shape (the solid line in Fig. 2) for various schemes of the electronic transitions. The curve of $N_B(t)$, in contrast, differs for the different schemes (the solid lines in

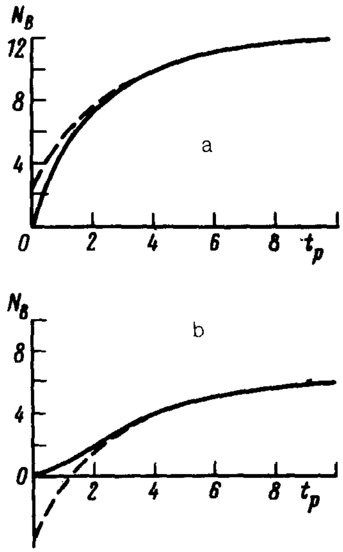

FIG. 3. Concentration of the ground state versus the duration of the filling pulse.

Fig. 3, a and b), since there are opposite signs (in the case $k_B > k_{AB}$) on the second term in expression (3). The dashed lines in Figs. 2 and 3 are plots of Eqs. (2) and (3) under the condition $\exp(-k_1 t) = 0$. Under the conditions $t \gtrsim k_{AB}^{-1} \gg k_1^{-1}$, the curves shown by the solid and dashed lines coincide, and this circumstance can be utilized to determine k_{AB} during the analysis of experimental data.

We have used the expressions derived here, (2) and (3), to study a bistable radiation-induced defect in n-type zone-refined silicon. Samples with a resistivity ~ 80 $\Omega \cdot$cm were bombarded with protons with an energy of 7.8 or 100 MeV. As in the case of γ-ray bombardment,[4] we observed two states of a defect, with thermal-ionization energies $E_t = 0.13 \pm 0.01$ eV and $E_t = 0.20 \pm 0.02$ eV. The length of the filling pulse was varied over the interval $t_p = 0.1$–100 μs. It was found that the concentration of the $E_t = 0.13$-eV states varies as a function of t in accordance with expression (2). This state is therefore metastable. The behavior of the concentration of the $E_t = 0.20$-eV state as a function of t is described by expression (3), which describes the formation of the ground state of a defect for the first configuration diagram (Fig. 1a). The coefficient which characterizes the reorganization from the metastable state to the ground state is an exponential function of the temperature: $k_{AB} = \nu \exp(-E_{AB}/kT)$, where $\nu = 1.4 \times 10^{12}$ s^{-1}, and $E_{AB} = 0.15$ eV.

In summary, theoretical expressions (2) and (3) can be compared with experimental data to reveal qualitative and quantitative characteristics of a bistable defect.

[1)]The initial conditions correspond to a large repetition period of the filling pulses in an experiment: $t_f \gg g^{-1}$.

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