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Electrical and Optical Characterization of Thermal Donors in Silicon

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Presently it is considered that the thermal donors (TD), formed in Si: O crystals at $T \lesssim 800$ K, are helium-like centers with the shallow levels $E_1 = E_c - (0.05 \text{ to } 0.07)$ eV and $E_2 = E_c - (0.12 \text{ to } 0.16)$ eV /1, 2/. However, such a picture of the electronic structure of TD is not exactly accurate. It is shown in /3, 4/ that two types of donor centers formed at early stages of thermal treatment n-Si:O at $T < 800$ K are configurationally bistable and can exist in four states: D_A^0, D_B^0, D_B^+, D_B^{++}, where the indexes A and B denote different center configurations (Fig. 1). In the A configuration electrons are strongly bound with the center (the photoionization energy of the defects exceeds the energy gap). At the same time, the B configuration is characterized by a small binding energy of the electrons to the neutral ($\Delta E_1 \approx 0.07$ eV) and singly ionized ($\Delta E_2 \approx 0.15$ eV) centers.

It has been found /3, 4/ that bistable thermal donors (BTD) are an Anderson system with $U < 0$. An important feature of these defects is the occupancy level E(o/++) /5/. For BTD-1 $E(o/++) \approx E_c - 0.32$ eV, for BTD-2 $E(o/++) \approx E_c - 0.22$ eV /4/. Under equilibrium conditions when the Fermi level E_F is lower than E(o/++) the basic state of BTD is D_B^{++}, while at $E_F > E(o/++)$ it is D_A^0. However, in the latter case even relatively weak above-band-gap illumination at $T \geq 100$ K gives rise to a change of the BTD configuration: as a result of the trapping of a non-equilibrium hole the center transforms from the D_A^0 state to the D_B^+ one and then, as a result of the thermal emission of the second electron, to D_B^{++}. The rate of the reverse process is small even at $T \approx 300$ K /3, 4/ which allows to "freeze" BTD in the B configuration and to realize the metastable states D_B^0 and D_B^+. On the other hand, illumination of the crystal containing BTD

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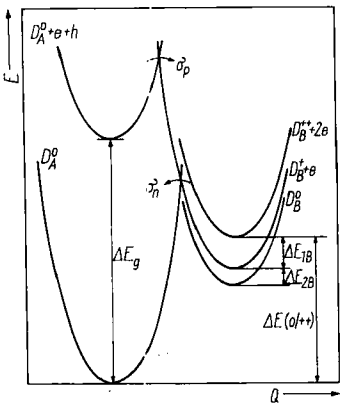

Fig. 1. Configuration-coordinate diagram for the bistable TD. ΔE_g band gap; $\Delta E(o/++) = E_c - E(o/++)$; ΔE_{1B} and ΔE_{2B} binding energies of the electrons on the neutral and singly ionized centers in configuration B

in the D_A^o state at sufficiently low temperature does not lead to a change of the defect configuration due to the presence of a barrier for hole trapping (see Fig. 1).

The above mentioned properties of BTD allow, using different regimes of cooling, to investigate the optical characteristics of BTD at low temperatures both in the A and B configurations. It can be expected that in the B configuration these centers are optically active in the range from 400 to 1200 cm^{-1} as other TD types (see /6, 7/). In this connection, we attempted to identify BTD by the IR absorption technique and to compare the obtained results with electrical measurement data.

Czochralski grown n-Si samples ($\varrho \approx 2\ \Omega$ cm) with concentrations of oxygen $[O] = 8 \times 10^{17}$ cm^{-3} and carbon $[C] = 10^{16}$ cm^{-3} were used. The samples were heat treated at 375 °C during 1 to 50 h. We measured the temperature dependences of the Hall constant (T_m = 77 to 400 K) and IR absorption in the range from 400 to 1200 cm^{-1} (T_m = 20 K).

The results of the electrical measurements are given in Fig. 2 in the form of $Y = kT\Delta(n_{ht} - n_{in})/\Delta F$ as a function of F, where $F = E_c - E_F$, n_{in} and n_{ht} are the concentrations of charge carriers before and after the heat treatment, respectively. The Y(F) value was determined by numerical differentiation of the experimental dependences of n(T) using the technique described in /8/. Y(F) has a maximum when the Fermi level crosses the occupancy levels of defects /8, 9/. In curve 1 (Fig. 2), obtained from the equilibrium dependence n(T), four bands with maxima at $F_{m1} \approx 0.07$, $F_{m2} \approx 0.15$, $F_{m3} \approx 0.22$, $F_{m4} \approx 0.32$ eV were observed. The half-widths of the first and second bands are $\delta F \approx 3.5$ kT (T_{m1} = 101 K, T_{m2} = 195 K), which is characteristic of the usual defects /9/. The amplitudes of these bands, proportional to the concentration of the levels ($Y_m = (1/4)N$), are equal to each other which is evidence

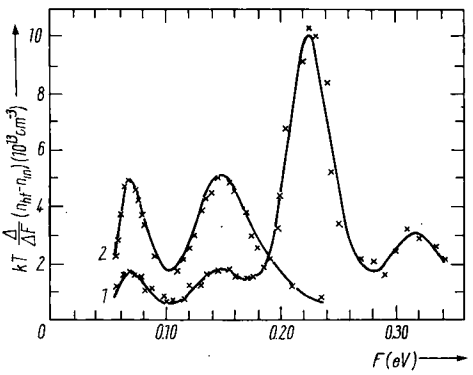

Fig. 2. $kT\Delta(n_{ht} - n_{in})/\Delta F$ as a function of the Fermi level position in n-Si subjected to heat treatment at 375 °C for 50 h; (1) measurements in darkness, (2) under weak illumination

of the fact that these two states belong to the usual double TD defects. The half-widths of the third and fourth bands are $\delta F \approx 1.8$ kT ($T_{m3} \approx 275$ K, $T_{m4} \approx 386$ K). This is a characteristic feature of the defects with $U < 0$ /9/, i.e. the levels $E_c - 0.22$ and $E_c - 0.32$ eV are the occupancy levels E(o/++) BTD-2 and BTD-1, respectively.

Curve 2 (Fig. 2) obtained from n(T) measurements under weak external illumination shows no deep levels. In this case the concentration of shallow levels (0.07 and 0.15 eV) increase by an order of magnitude equal to the sum of concentrations of deeper levels (for centers with $U < 0$ $Y_m = N$). Consequently, the illumination of the sample leads to the total transformation of BTD-1 and BTD-2 into the B configuration.

The IR absorption spectra of the same sample are shown in Fig. 3. In the spectrum of the crystal cooled under illumination a series of absorption bands (a, b, c, d, e), due to the transition from the ground state to the excited states of five neutral TD are observed /6, 7/. When the sample was cooled in darkness after previous exposure at 300 K, the bands of the a-series disappeared (Fig. 3, curve 2). After a long-time exposure ($t \gtrsim 5$ h) of the sample in darkness at 270 K a noticeable reduction by a factor of 3 of the b-series intensity is revealed. This allows to conclude that the a- and b-series belong to the bistable TD.

The comparison of the concentration of the BTD-1 and BTD-2 centers (see Fig. 2) with the intensities of the corresponding bands indicates that the a-series is related to BTD-1, and the b-series to BTD-2. This identification accounts for the difference between the spectra 2 and 3 in Fig. 3. In the investigated crystals at T = 300 K the Fermi level is at $E_c - 0.25$ eV, i.e. it is located above the occupancy level of BTD-1 but lower than that of BTD-2. In this case the equilibrium configuration of BTD-1 will be the optically inactive

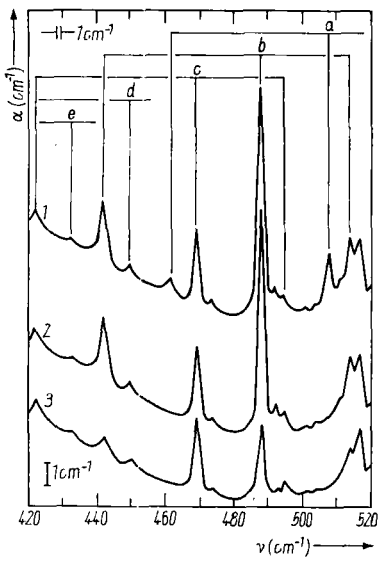

Fig. 3. Absorption spectra of the same material as shown in Fig. 2, measured at a sample temperature of 20 K; (1) cooling under illumination, (2), (3) cooling in darkness after exposure at 300 and 270 K, respectively

configuration A (a-series disappears) and BTD-2 - the configuration B, which remains when the sample is cooled to T_m = 20 K. When the temperature of the exposure is T = 270 K, the Fermi level shifts to E_c - 0.2 eV and the main part of BTD-2 transforms to the D_A^0 state for t > 5 h, which gives rise to an essential reduction of the intensity of the b-series lines.

Thus, from the results obtained in this note it follows that two of nine types of double thermal donors found earlier /6, 7/ are bistable. The presence of two stable configurations of TD should be taken into account in investigating the kinetics of the formation of these centers as well as in developing a microscopic model.

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