Spin-correlated electron transfer along broken bonds in semiconductors

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We investigate the characteristics of diffusive transfer of singlet and triplet centers along broken bonds in semiconductors. We show that this transfer takes place because of spin-correlated adiabatic small-polaron hopping. Using the kinetic equation for electron transfer in narrow bands, we calculate the probability of spin-correlated hopping in isotropic and anisotropic systems of broken bonds. We obtain an exact solution for the probability of variable-range hopping which goes beyond the framework of the "Mott logarithm." We show that thermalization of carriers in a narrow band stimulates a change in the effective dimensionality of the system of broken bonds. The diffusion coefficient for polarized triplet centers is significantly dependent on the magentic states of the broken bond system. These results are used to interpret experimental data obtained in the course of this work on the optical polarization of nuclear moments (OPNM) in plastically-deformed silicon. We demonstrate the important role of the spin correlation length and the effective residence time of a triplet center on a broken bond in OPNM processes. Magnetic ordering of dislocations is observed in the broken bond system when conditions are fulfilled for spin-correlated transfer of polarized triplet centers.

INTRODUCTION

Dislocation-induced broken bonds (DBB) in plastically-deformed single-crystal semiconductors are anisotropic defects with positive correlation energies.[1–6] Because of this, the electronic energy spectrum of a DBB is that of a Mott-Hubbard narrow-band insulator[3,6,7] (Fig. 1). In addition to the singlet one-electron excitation band (*S*-centers), the triplet-excitation band (*T*-centers) of the DBB system also plays a significant role in the dislocation-mediated recombination of non-equilibrium carriers.[5,6,8] The presence of these bands gives rise to the following spin-dependent effects: (1) the dependence of the polaron tunneling factor, which corresponds to a structural rearrangement of the broken bonds, on the charge and spin state of the DBB[6]; (2) selective trapping of nonequilibrium carriers at the magnetic sublevels of the *T*-center which are characterized by different projections of the total spin, leading to the appearance of a nonequilibrium spin polarization associated with excited triplet states of the DBB[5,6,9]; (3) spin-correlated transfer of the polarized *T*-centers along the dislocation chain, which induces a nonequilibrium polarization of the background electrons of the DBB (the *D*-center band; see Ref. 6); this polarization is reflected in spin-dependent recombination (SDR) and optical polarization of nuclear moments (OPNM) in the host semiconductors.[5,6,8,10,11]

The nonequilibrium polarization of DBB significantly exceeds the corresponding Boltzmann value even in the case of strong magnetic fields, and influences the rate at which the states of *S* and *T* centers on the dislocation chains are populated. A consequence of this is the observed giant values of SDR and OPNM.[6,8,9]

The goal of this paper is to investigate the distinctive features of spin correlated transfer of *S* and *T* centers in a DBB system, which is an intermediate step in the process of recombination of nonequilibrium charge carriers mediated by dislocation chains; because of effects associated with magnetization of the background DBB electrons, this process influences the temperature and field dependences of the SDR and OPNM in a significant way. The interval of characteristic times over which transfer of *S* and *T* centers in the DBB system is important is bounded from below by the average lifetime of a band charge carrier relative to trapping by the DBB, and from above by the average time for annihilation reactions of the *S* and *T* centers with nonequilibrium holes trapped by the dislocations (see Ref. 6) which complete the recombination process.

In Sec. 2 we show that the mutual coupling of the multiplet spin correlations and the electron-phonon interaction (EPI) at each DBB leads to spin-correlated tunneling of electrons between broken bonds, and that this coupling is the reason for spin-correlated thermally-activated transfer in semiconductor dislocation systems. In Sec. 3 we give a derivation of the kinetic equation for electron transfer in a narrow band due to spin-correleated adiabatic small-polaron hopping, taking into account thermalization effects. In Sec. 4 we present results of calculations of the probability for thermally-activated small-polaron hopping in isotropic and anisotropic DBB systems; we obtain an exact expression for the variable-range hopping probability, which improves on the "Mott logarithm" approximation. We show that thermalization of carriers in a narrow band stimulates a change

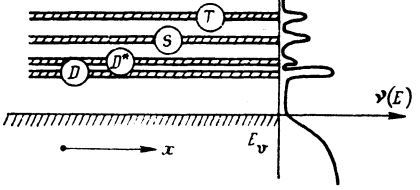

FIG. 1. Sketch of narrow bands formed by the various DBB states in the forbidden gap of silicon as a function of the Cartesian coordinate *s* and the corresponding density of states $\nu(E)$.[1]

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in the effective dimensionality of the thermally-activated diffusive transport. In Sec. 5 we present the results of our investigation of the effects of magnetization of the DBB background electrons under conditions of spin-correlated transfer of polarized T-centers, which is used in interpreting the DBB experimental data.

2. MULTIPLET SPIN CORRELATION AND ELECTRON-PHONON INTERACTION IN SEMICONDUCTOR DBB SYSTEMS

Because electron states at the DBB are strongly localized due to disordered strain and polaron effects, spin-correlated electron transfer in the narrow bands (Fig. 1) is thermally activated.[6] S- and T-centers are small polarons, because the polaronic and bipolaronic shifts for carriers trapped on DBB significantly exceed the width of the Mott-Hubbard insulator bands (Fig. 1), which is of the same order of magnitude as the mean-square fluctuations associated with the strain disorder (B_0). Therefore, thermally-activated electron transfer in the DBB system takes place because of intercenter adiabatic hopping of small polarons (SP).

In order to describe the spin-correlated transfer we must take into account the mutual coupling of the multiplet spin correlations and the EPI at each separate broken bond. The Hamiltonian of the DBB system[1] is conveniently represented by using the projection operators $\beta_{j\alpha} = \beta_{j\alpha}^2$ of its various charge and spin states (α and j are indices for the state and bond number of the DBB):

$$\mathcal{H}_0=\sum_j \hbar_j, \quad \hbar_j=\frac{P_j^2}{2M_0}+\frac{\varkappa}{2}Q_j^2+\sum_\alpha \beta_{j\alpha}(E_{j\alpha}-Q_jF_\alpha), \tag{1}$$

where

$$E_{j\alpha}=\begin{cases}\begin{pmatrix}E_{j0}\\ E_{j1}\end{pmatrix}, & n_j=1, \quad \alpha=\begin{pmatrix}D\\ D^\cdot\end{pmatrix},\\ 2E_{j0}+U, & n_j=2, \quad \alpha=S,\\ E_{j0}+E_{j1}+U_M, & n_j=2, \quad \alpha=(T, M=0, \pm1),\end{cases}$$

$$U_M=\begin{cases}U_1, & M=0,\\ U_2, & M=\pm1,\end{cases} \tag{2}$$

$$F_\alpha=\begin{cases}F_0, & n_j=1, \quad \alpha=\begin{pmatrix}D\\ D^\cdot\end{pmatrix},\\ F_S=2F_0+F_1, & n_j=2, \quad \alpha=S,\\ F_T=2F_0+F_2, & n_j=2, \quad \alpha=(T, M=0, \pm1),\end{cases}$$

P_j and Q_j are the canonical momentum and coordinate of the DBB with index j; M_0 and $\varkappa$ are the effective mass and coupling constant of the bond; $n_j = 1,2$ denotes the total number of electrons on the center; E_{j0} and E_{j1} are the random bare single-electron energies of the D-centers, which are distributed uniformly along the dislocation chains in the energy interval B_0 due to the strong strain disorder (see, e.g., Refs. 12, 13); $E_{j\alpha}$ and F_α are the electronic part of the DBB energy and the EPI constant for the state α; and M is the triplet spin projection. The DBB correlation energies U, U, and U_2, which depend on the total charge and spin of the DBB, and the EPI constants at the DBB F_0, F_1, and F_2, were introduced in Ref. 6. It should be noted that the difference in the values of the EPI constants F_S and F_T [see (2)] for the singlet and triplet states of the DBB is connected with the fact that by virtue of the Pauli principle the spatial parts of the electronic wave functions are different in these two states.

The electron and phonon variables in the Hamiltonian $\mathcal{H}_0$ are decoupled by the following polaron canonical transformation, which also includes a bipolaron transformation for the two-electron states ($n_j = 2$):

$$\mathcal{U}=\prod_{j,\alpha}(u_{j\alpha})^{\beta_{j\alpha}}, \quad u_{j\alpha}=\exp[\gamma_\alpha(c_j^+-c_j)]=\exp\left(-\frac{i}{\hbar}P_jQ_\alpha\right),$$

$$\gamma_\alpha=\frac{F_\alpha Q_{min}}{\hbar\omega_0}, \quad \omega_0^2=\frac{\varkappa}{M_0}, \quad Q_{min}=\left(\frac{\hbar}{2M_0\omega_0}\right)^{1/2}, \quad Q_\alpha=\frac{F_\alpha}{\varkappa}, \tag{3}$$

where c_j^+ and c_j are creation and annihilation operators for the local phonon mode of the jth DBB with characteristic frequency ω_0. The result has the form

$$\mathcal{H}_0=\mathcal{U}H_0\mathcal{U}^{-1},$$

$$H_0=\sum_j h_j, \quad h_j=\sum_\alpha \beta_{j\alpha}\mathcal{E}_{j\alpha}+\hbar\omega_0(c_j^+c_j+1/2), \tag{4}$$

$$\mathcal{E}_{j\alpha}=E_{j\alpha}-W_\alpha, \quad W_\alpha=\bar{N}_\alpha\hbar\omega_0>0, \quad \bar{N}_\alpha=\gamma^2\alpha.$$

Here Q_α and W_α are the polaron ($n_j = 1$) and bipolaron ($n_j = 2$) coordinate and energy shifts, respectively; $\bar{N}_\alpha$ is the Huang-Rhys factor for the state α; $\mathcal{E}_{j\alpha}$ as opposed to $E_{j\alpha}$ in (2) denotes the ground-state energy of a polaron ($n_j = 1$) and a bipolaron ($n_j = 2$) at a DBB, which equal the corresponding thermoionization potentials with opposite sign.

In studying the transfer of correlated electrons ($n_j = 2$, $\alpha = S$ or T) in the DBB system it is also necessary to investigate a decoupling procedure analogous for (4); however, this procedure will involve variables only of the correlated electrons of the DBB, while the variables of the background electrons are excluded. To implement this procedure, we change from the bipolaronic canonical transformation to the usual polaronic one, which corresponds to relaxation of a two-electron center which is being singly ionized. The reduced polaronic canonical transformation we seek has the form

$$\hat{\mathcal{U}}=\prod_{j,\alpha}(u_{j\alpha})^{\beta_{j\alpha}}(u_{j0}^{-1})^{\beta_{j0}}, \quad n_j=2, \quad \alpha=S \text{ or } T, \tag{5}$$

where the index "0" refers to the background electrons ($n_j = 1, \alpha = D$); $\beta_{j\alpha}$ and β_{j0} are projection operators for the two-electron and one-electron states of the DBB, respectively: $\hat{\mathcal{U}}$ is a product of factors of the form (see, e.g., Ref. 14)

$$\exp\left[-\frac{i}{\hbar}P_j(\beta_{j\alpha}Q_\alpha-\beta_{j0}Q_0)\right], \tag{6}$$

which correspond to spin-dependent translation operators for the jth oscillator at the value of the polaron shifts.

According to Ref. 6, the correlated electrons of the DBB are described by one-electron wave functions which take into account the multiplet spin correlations. The spin parts of the latter χ_s ($\alpha = S$) and χ_M ($M = 0, \pm 1; \alpha = T$), which depend on the electron spin projection σ and on the spin variables ξ_j of the background electrons of the jth DBB, are determined by the relations

$$\left.\begin{matrix}\chi_S\\ \chi_0\end{matrix}\right\}=2^{-1/2}[\xi_j u_\downarrow(\sigma)\mp(1-\xi_j)u_\uparrow(\sigma)], \tag{7}$$

$$\chi_{+1}=\xi_j u_\uparrow(\sigma), \quad \chi_{-1}=(1-\xi_j)u_\downarrow(\sigma),$$

where u_σ are the usual spinors. The spin projection σ_j' of background electron is related to the parameter $\xi_j = (1 + \sigma'_j)/2 = 0,1$.

Based on (5)–(7), it is easy to show that the usual hopping term $\mathscr{H}_1$ in the original Hamiltonian for the DBB electrons (for simplicity we will neglect the contribution from two-electron hopping) can be written in the form ($\alpha = S$ or T)

$$\mathscr{H}_1=\hat{\mathscr{U}}H_1\hat{\mathscr{U}}^{-1}, \quad H_1=\sum_{i,j,\alpha}{}' \eta_\alpha(\xi_i,\xi_j)I_{ij}^{(0)}v_{i\alpha}^{-1}v_{j\alpha}b_{i\alpha}^{+}b_{j\alpha}, \tag{8}$$

where

$$v_{j\alpha}=\exp[(\gamma_\alpha-\gamma_0)(c_j^{+}-c_j)]$$

$$=\exp\left[-\frac{i}{\hbar}P_j(Q_\alpha-Q_0)\right], \quad n_j=2, \tag{9}$$

$$\eta_\alpha(\xi_i,\xi_j)=\begin{cases} {}^1/_2[\xi_i\xi_j+(1-\xi_i)(1-\xi_j)], & \alpha=S \quad \text{or} \quad (T,M=0),\\ \xi_i\xi_j, & \alpha=(T,M=1),\\ (1-\xi_i)(1-\xi_j), & \alpha=(T,M=-1). \end{cases} \tag{10}$$

Here $I_{ij}^{(0)}$ is the bare resonance integral, which depends on the radius vector $\mathbf{R}_{ij}$ connecting DBB with indices i and j; $b_{j\alpha}^{+}$ and $b_{j\alpha}$ are creation and annihilation operators for a correlated electron on a DBB in state α.[6]

The energy ($\hbar\omega_0$) of local phonons associated with the defect vibrational modes of the DBB can exceed the Debye energy $\hbar\omega_0$ which determines the maximum of the spectrum of the three-dimensional acoustic phonons near a semiconductor dislocation ($\hbar\omega_0 > \hbar\omega_D > k_B T$).[6] Therefore the spin-correlated thermally-activated hopping of SP along the dislocation chains has an adiabatic character, i.e., it proceeds by weak inelastic tunneling between equilibrium positions in the lattice without exciting local phonons of the defect modes. In practice, the amplitude of such hops is proportional to the effective hopping integral, which is obtained from (8) after averaging over the thermal distribution of local phonon modes of the DBB. Using obvious relations for thermal averages for arbitrary i and j:

$$\langle v_{i\alpha}^{-1}v_{j\alpha}\rangle=\exp[-\bar{N}_{\alpha0}(2\langle N\rangle+1)]\approx K_0(Q_0-Q_\alpha),$$
$$\bar{N}_{\alpha0}=(\gamma_\alpha-\gamma_0)^2, \quad \langle N\rangle=[\exp(\hbar\omega_0/k_BT)-1]^{-1}\ll 1, \tag{11}$$

we obtain

$$\langle H_1\rangle=\sum_{i,j,\alpha}{}' I_{ij,\alpha}b_{i\alpha}^{+}b_{j\alpha}, \tag{12}$$

$$I_{ij,\alpha}(\xi_i,\xi_j)=\eta_\alpha(\xi_i,\xi_j)I_{ij}^{(0)}K_0(Q_0-Q_\alpha),$$

where K_0 is the spin-dependent tunneling factor K_N introduced in Ref. 6 evaluated at zero phonon number for the mode of the final DBB state ($N = 0$).

In agreement with the results of Holstein,[15,16] the effective spin-dependent hopping integral (12) for a narrow band of small polarons and bipolarons is proportional to the tunneling factor. Consequently, the probability of spin-correlated adiabatic hopping of SP between DBB, as in the problem without spin correlation (see, e.g., Refs. 16, 17), depends quadratically on the tunneling factor. Physically, this dependence reflects the fact that the inter-site hopping of a charge carrier is accompanied by simultaneous tunneling-induced structural rearrangements of the original and final centers.

It must be emphasized that according to (10), (12) both intercenter tunneling hops and thermally-activated hopping of electrons between the DBB (Sec. 3) are spin-correlated: as a consequence of the local spin correlation (1), (2) there arises a dependence of the hopping probability on the spin state of the DBB system. The following condition serves as a criterion for existence of such correlation: spin correlation exists when the probability of intercenter hopping, taking into account (12) (Sec. 3), exceeds the probability of spin relaxation at the DBB, as occurs in silicon.[5,6] The advantage of using the single-electron wave functions introduced in Ref. 6, which include local spin correlation at the DBB (7), lies in the possibility of reducing a three-body problem, i.e., the intercenter hopping of a correlated electron when a background electron is present at both the initial and final centers to interact with it, to the single-electron problem (7), (12) with subsequent averaging over the spin states (ξ_j) of the background electron system at the core of the edge dislocation.

The overlap integral (12) depends on distance in an essentially exponential fashion. Therefore the spin-correlated transfer is characterized by the final-state correlation length—the diffusion length for charge carriers in the DBB system, which corresponds to the spin-lattice relaxation time of the background electrons (Sec. 5.2).

3. KINETIC EQUATION FOR ELECTRON TRANSFER IN A NARROW BAND

A fundamental consequence of the spin correlation at broken bonds is the fact that for an S- or T-center with fixed spin projection certain sites in the DBB system are forbidden on the basis of spin: $\eta_\alpha = 0$ in (10), (12). Calculations of the probability of spin-correlated adiabatic hopping of SP between states of the DBB $\alpha = S$ or T are based on the use of the pairing approximation[18–21] for single-electron wave functions of correlated electrons of the DBB.[6] In order to simplify the notation, in what follows we omit the state index α and the spin variables $\{\xi_j\}$ [see (12)], although it is necessary to average over these variables at the end of the calculation. In the limit of weak overlap [Eq. (12)] the wave functions of a correlated electron in the spin–dependent pairing approximation have the form

$$\varphi_i'=\varphi_i\mp(|I_{ij}|/\Delta_{ij})\varphi_j, \quad \varphi_j'=\varphi_j\pm(|I_{ij}|/\Delta_{ij})\varphi_i, \quad X_{ij}\lessgtr 0,$$
$$\Delta_{ij}=(X_{ij}^2+4I_{ij}^2)^{1/2}\gg|I_{ij}|, \tag{13}$$

where the energy difference Δ_{ij} of antibound and bound states in a pair takes into account quantum-mechanical level repulsion; the probability distribution function for the difference $X_{ij} = \mathscr{E}_i - \mathscr{E}_j$ of random deformation potentials at the centers is expressed by the quantity B_0 introduced above (Sec. 2), and has a triangular form

$$\mathscr{P}(X)=\theta(B_0-|X|)B_0^{-1}(1-|X|/B_0), \tag{14}$$

$\theta(X)$ is the Heaviside function.

Let $n_i(E)$ be the distribution of correlated electrons at the ith DBB, where the carrier energy E varies within a narrow band of width B. Then the arrival (upper sign) and departure (lower sign) probabilities for adiabatic hopping of an SP referred to a state with indices (i, E) have the form

$$\pm 2\pi \sum_{j,\mathbf{q}} |C_q|^2 |\langle \varphi_i' | e^{i\mathbf{qr}} | \varphi_j' \rangle|^2 \delta(\Delta_{ij}(X_{ij})/\hbar - \omega_q)$$
$$\times \{\theta(X_{ij})(\mathcal{N}_q + {}^1/_2 \mp {}^1/_2)[n_j(E-\Delta_{ij}) - {}^1/_2 \pm {}^1/_2]$$
$$+\theta(-X_{ij})(\mathcal{N}_q + {}^1/_2 \pm {}^1/_2)[n_j(E+\Delta_{ij}) - {}^1/_2 \pm {}^1/_2]\}, \quad (15)$$

where $|C_q|^2 = \Xi^2 q/2V\rho v_s \hbar$ is the square of the matrix element for the deformation-acoustic (DA) electron-phonon interaction, Ξ is the deformation potential constant, $\omega_q = v_s q$ and $\mathcal{N}_q$ are the frequency and occupation number of phonons with quasimomentum $\mathbf{q}$, v_s is the longitudinal sound velocity, ρ is the density, and V is the normalization volume. It should be emphasized that the interaction of electrons with local modes of the DBB in (15) is included exactly through the reduction transformation (5), and in this sense the intercenter transitions are single-phonon.

Within the pairing approximation (13), the square of the total matrix element averaged over angle in (15) coincides in form with the same quantity where spin correlations are absent[19] (μ is the cosine of the polar angle):

$$M_{ij}(q, X_{ij}) = \int_{-1}^{1} \frac{d\mu}{2} |\langle \varphi_i' | e^{i\mathbf{qr}} | \varphi_j' \rangle|^2 \approx \frac{2I_{ij}^2}{\Delta_{ij}^2}. \quad (16)$$

Here we have used bounds on the energy transfer during an intercenter hop in the form

$$\hbar\omega_q \sim \Delta_{ij} \leqslant \hbar\omega_D, \quad qa \approx \frac{\omega_q}{v_s} a \leqslant \frac{\omega_D a}{v_s} < 1, \quad R_{ij} > a, \quad qR_{ij} > 1, \quad (17)$$

where a is the localization radius of the basis states of the DBB. We cast (15) in the form of an integral over energy transfer:

$$\pm \sum_j \int d\varepsilon \, w_{ij}^{\pm}(\varepsilon, X_{ij})[n_j(E-\varepsilon) - {}^1/_2 \pm {}^1/_2], \quad (18)$$

where $w_{ij}^{\pm}$ is the differential probability of arrival and departure for a given site i. The averaging over the deformation disorder (14), which we denote with an overline, reduces to replacing the probability in (18) by corresponding quantities of the form

$$w_{ij}^{+}(\varepsilon) = \overline{w_{ij}^{+}(\varepsilon, X)} = \frac{\Xi^2 |\varepsilon|^3}{2\pi\rho v_s^5 \hbar^4} \mathcal{M}_{ij}(\varepsilon)[\theta(\varepsilon)\mathcal{N}(\varepsilon)$$
$$+\theta(-\varepsilon)(\mathcal{N}(|\varepsilon|)+1)], \quad (19)$$
$$w_{ij}^{-}(\varepsilon) = \overline{w_{ij}^{-}(\varepsilon, X)} = w_{ij}^{+}(-\varepsilon) = w_{ji}^{+}(\varepsilon),$$
$$\mathcal{N}(\varepsilon) = [\exp(\varepsilon/k_B T) - 1]^{-1},$$
$$\mathcal{M}_{ij}(\varepsilon) = \int dX \, \mathcal{P}(X) M_{ij}\left(\frac{|\varepsilon|}{\hbar v_s}, X\right) \theta(\pm X) \delta(\Delta_{ij}(X) - |\varepsilon|)$$
$$\approx \frac{2I_{ij}^2}{|\varepsilon| B_0} [(\varepsilon^2 - 4I_{ij}^2)^{-1/2} - B_0^{-1}]. \quad (20)$$

It is important to explain the bounds on the energy transfer ε which arise in the course of obtaining (20): they are a consequence of the properties of the distribution (14), and have the form

$$2|I_{ij}| \leqslant |\varepsilon| \leqslant (B_0^2 + 4I_{ij}^2)^{1/2}. \quad (21)$$

According to (18)–(20), the kinetic equation which describes spin-correlated diffusive transfer of adiabatic SP in narrow bands of S- and T-centers on broken bonds has the form

$$\dot{n}(E, \mathbf{r}) = -W(E) n(E, \mathbf{r}) + \int d\varepsilon [w(\varepsilon) + D(\varepsilon) \nabla^2] n(E-\varepsilon, \mathbf{r}),$$
$$W(E) = \sum_j{}' \int d\varepsilon \, w_{ij}^{+}(-\varepsilon), \quad (22)$$

where the effective arrival probability summed over sites and the differential (in energy transfer) diffusion coefficient are

$$w(\varepsilon) = \sum_j{}' w_{ij}(\varepsilon), \quad D(\varepsilon) = \frac{1}{2d} \sum_j{}' R_{ij}^2 w_{ij}^{+}(\varepsilon), \quad (23)$$

d is the dimension of the space. The limits of integration in (22) are determined not only by the boundaries of the Brillouin zone, but also by the energy E of carriers in the narrow band, i.e.,

$$\varepsilon_{min} = \max(-\hbar\omega_D, E-B), \quad \varepsilon_{max} = \min(\hbar\omega_D, E). \quad (24)$$

It is obvious that the sum of the first two terms on the right side of Eq. (22) is the usual DA phonon collision integral, which describes the local thermalization of the correlated electrons. The structure of the diffusion term in (22), taking into account (24), allows us to draw the conclusion that the effective diffusion velocity along the broken bonds in semiconductors depends significantly on the average energy of the electron distribution in the narrow band, i.e., the effective diffusion coefficient changes in the process of thermalization; this fact is very important from the point of view of applications (Sec. 5). Equation (22) for $d = 1$ coincides in form with the diffusion equation for spinless hopping transport in the absence of polaron effects obtained in Ref. 22 within the framework of the one-dimensional theory of electron localization at nonzero temperatures.

4. SPIN-DEPENDENT ADIABATIC HOPPING OF SMALL POLARONS

4.1 Isotropic DBB systems

In order to describe the spin-correlated transport of adiabatic SP along broken bonds, it is necessary to evaluate sums of the form (23). The calculations reduce to determining the energy-dependent probability for variable-range hopping,[19–21] Such sums are calculated approximately to logarithmic accuracy; to leading order, the resulting transport quantities contain the "Mott logarithm" to a power which equals $d-1$ for $w(\varepsilon)$ and $d+1$ for $D(\varepsilon)$. For our purposes, this approximation is insufficient, because the transferred energy ε can vary over wide limits; it is especially important to take this into account in studying the thermalization which accompanies transport along the broken bonds.

The summation over sites in (23) can be treated like an averaging over distances between bonds of the DBB. In transforming the sum over sites into an integral over bond distance R it is necessary to cut off a certain region in the vicinity of the origin whose size and shape is determined on one hand by the geometric characteristics of the overlap integral, and on the other hand by the ratio of atomic lattice constants. In the case of a spherically-symmetric overlap integral

$$I_{ij}\to I(R)=I_0\exp(-R/a),\quad I_0<0,\tag{25}$$

the cut-off region is a sphere with radius R_0 on the order of the distance between broken bonds a_0. The quantity (23) can be cast in the form

$$w(\varepsilon)=\mathscr{F}(\varepsilon)J_{d-1}(\varepsilon),\quad D(\varepsilon)=\frac{1}{2d}\mathscr{F}(\varepsilon)J_{d+1}(\varepsilon),$$

$$\mathscr{F}(\varepsilon)=\frac{d\pi^{d/2-1}}{a_0{}^d\Gamma(1+d/2)}\frac{\Xi^2}{\rho v_s{}^5\hbar^4B_0}\{\theta(\varepsilon)\mathscr{N}(\varepsilon)\tag{26}$$

$$+\theta(-\varepsilon)[\mathscr{N}(|\varepsilon|)+1]\},$$

where $\Gamma(x)$ is the gamma function. As a result, the problem reduces to calculating the integral

$$J_n(\varepsilon)=\varepsilon^2\int\limits_{R>R_0}R^n\,dR\,I^2(R)\{[\varepsilon^2-4I^2(R)]^{-1/2}-B_0^{-1}\}.\tag{27}$$

The limits of integration are determined by the region of variation of ε; in agreement with (21) we have three significant regions:

$$\begin{aligned}&\text{(I)}\quad 0<|\varepsilon|\leqslant\varepsilon_1,\quad R_\varepsilon\leqslant R<\infty,\\&\text{(II)}\quad \varepsilon_1\leqslant|\varepsilon|<B_0,\quad R_0\leqslant R<\infty,\\&\text{(III)}\quad B_0\leqslant|\varepsilon|<B,\quad R_0\leqslant R<R_\varepsilon',\end{aligned}\tag{28}$$

where the following notation is introduced:

$$\varepsilon_1=\max 2|I|=2|I_0|\exp(-R_0/a),\quad B=\max|\varepsilon|=(B_0^2+\varepsilon_1^2)^{1/2},$$

$$R_\varepsilon=a\ln\frac{2|I_0|}{|\varepsilon|},\quad R_\varepsilon'=a\ln\frac{2|I_0|}{(\varepsilon^2-B_0^2)^{1/2}}.\tag{29}$$

ε_1 is the energy corresponding to the maximum overlap at the dislocation chain; R_ε is the Mott logarithm.[21]

After the substitution $z=\exp[-2(R-R_\varepsilon)/a]$, the integral (27) is calculated exactly and is expressed in terms of derivatives of Euler's incomplete beta-function. Using a representation of these derivatives in terms of the hypergeometric function in the form of an infinite series, we have

$$J_n(\varepsilon)=\frac{1}{4}\varepsilon^4I_0^2\sum_{k=0}^{n}a_kR_\varepsilon^k,$$

$$a_k=(-1)^{n-k}\binom{n}{k}\left(\frac{a}{2}\right)^{n+k+1}[q_{n-k}(z_{max})-q_{n-k}(z_{min})],\tag{30}$$

$$q_m(z)=z\sum_{k=0}^{m}(-1)^{m-k}\binom{m}{k}(m-k)!\ln^kz\left(\frac{1}{|\varepsilon|}\zeta_{m-k}(z)-\frac{1}{B_0}\right),$$

$$\zeta_m(z)=\frac{1}{\pi^{1/2}}\sum_{n=0}^{\infty}\frac{\Gamma(n+1/2)}{(n+1)^m}\frac{z^n}{(n+1)!}.$$

According to (28), (29), the parameter $z_{\max}$ equals 1 in region I and $(\varepsilon_1/\varepsilon)^2$ in regions (II), (III), while $z_{\min}$ equals 0 in regions I, II, and $1-(B_0/\varepsilon)^2$ in region (III). The representation (30) is the expansion of the integral (27) in the Mott logarithm, and for very small ε (region I) the leading order of this logarithm gives the basic contribution; this coincides with the basic result of the theory of impurity-band conduction due to variable-range hopping.[19,20] In the theory of phononless hopping conductivity[21] the integration over ε is absent: $\varepsilon=\hbar\Omega$, where Ω is the frequency of the AC electric field.

As a consequence of (12), the tunneling-induced smallness of the quantity $|I_0|$ in (25) limits the applicability of the Mott-logarithm approximation to the very narrow region I, because ε_1 is much smaller than keT and $\hbar\omega_0$. Herein lies the principal difference between the spin-correlated transport of SP in a narrow band ($B\gtrsim B_0\gg\varepsilon_1$) under discussion here and the well-known theory of hopping conductivity. So as to clarify the character of the behavior of $J_n(\varepsilon)$ in the most important region (II) of variation of the transferred energy, it is sufficient to investigate (27) in the limit $|\varepsilon|\gg\varepsilon_1$. As a result, we obtain

$$J_n(\varepsilon)\approx I_0^2\left(|\varepsilon|-\frac{\varepsilon^2}{B_0}\right)\left(\frac{a}{2}\right)^{n+1}$$

$$\times\exp\left(-\frac{2R_0}{a}\right)\sum_{k=0}^{n}\frac{n!}{k!}\left(\frac{2R_0}{a}\right)^k\tag{31}$$

Taking into account (26), the behavior of $w(\varepsilon)$ and $D(\varepsilon)$ in region (II) for arbitrary n is described by the inverted parabola $(|\varepsilon|-\varepsilon^2/B_0)$. The approximation agrees well with the result of evaluating the integral (27) numerically (Sec. 2), excluding the very narrow boundary regions (II) and (III).

4.2. Anisotropic DBB systems

The real wave functions and overlap integrals on a DBB chain are anisotropic.[22] In addition, a system of semiconductor dislocations can be treated approximately as an anisotropic lattice of allowed sites. Each of these types of anisotropy can be taken into account in a common fashion if we generalize the results of the previous section after applying a scaling transformation to the lattice.

Let the overlap integral depend on the radius vector connecting any two DBB and not just on its absolute value:

$$I_{ij}\to I(\mathbf{R})=I_0\exp\left[-\left(\frac{X^2}{a_1^2}+\frac{Y^2+Z^2}{a_2^2}\right)^{1/2}\right],\quad a_1>a_2.\tag{32}$$

Let us also assume that the dislocations form a regular lattice on the average with a constant b_1 along the dislocation axis and a constant b_2 in the plane perpendicular to this axis. Obviously, there is no dependence on azimuthal angle in such a system; therefore, in passing from the summation over sites in (23) to an integration over bond lengths, we obtain in place of (27) an integral of the form

$$J_n'(\varepsilon)=\left(\frac{a_2}{a_1}\right)^2\varepsilon^2\int_{-1}^{1}d\mu\int\limits_{R'>R_0(\mu)}R'^n\,dR'\,I^2(R')$$

$$\times\{[\varepsilon^2-4I^2(R')]^{-1/2}-B_0^{-1}\}.\tag{33}$$

Here we have already performed the scale transformation $\mathbf{R}\to\mathbf{R}'(Y/Y'=Z/Z'=a_2/a_1)$, which transforms the overlap integral (32) to the isotropic form (25) with $a=a_1$. The transformed lattice constant in the plane perpendicular to the dislocation axis also changes: $b_2\to b_2'=(a_1/a_2)b_2$. The problem of calculating the integral over R' in (33) reduces to the problem (27) with the difference that the region of integration now depends on the polar angle ($\mu = \cos\theta$). This is related to the fact that in an anisotropic lattice it is necessary to cut off not a spherical but rather an ellipsoidal region in the vicinity of the origin, e.g.,

$$R_0(\mu) = R_0[\mu^2 + (1-\mu^2)/\gamma^2]^{-1/2}, \quad \gamma = b_2'/b_1 > 1, \quad R_0 \sim b_1. \tag{34}$$

It is easy to see that the angular dependence (34) leads to anisotropic spin-correlated transport of SP in the DBB system, i.e., to a dependence of the probability on the direction of hopping.

Analysis of the limits of integration in (33) based on relations (21) and (34) shows that the range of variation of ε in the present case is divided into five principal regions, and at the band edges there are two characteristic angular scales (μ_1 and μ_2):

$$\left.\begin{array}{lll} (\mathrm{I}') & 0 < |\varepsilon| \leqslant \varepsilon_2 & \\ (\mathrm{II}') & \varepsilon_2 < |\varepsilon| < \varepsilon_1 & |\mu| > \mu_1 \end{array}\right\} R_\varepsilon \leqslant R' < \infty,$$
$$\left.\begin{array}{lll} & & |\mu| < \mu_1 \\ (\mathrm{III}') & \varepsilon_1 \leqslant |\varepsilon| < B_0 & \end{array}\right\} R_0(\mu) \leqslant R' < \infty,$$
$$\left.\begin{array}{lll} (\mathrm{IV}') & B_0 < |\varepsilon| \leqslant \varepsilon_3 & \\ (\mathrm{V}') & \varepsilon_3 < |\varepsilon| < B & |\mu| > \mu_2 \end{array}\right\} R_0(\mu) \leqslant R' < R_\varepsilon', \tag{35}$$

where the definition (29) is used for $a = a_1$:

$$\varepsilon_2 = 2|I_0| \exp(-\gamma R_0/a_1) < \varepsilon_1, \quad \varepsilon_3 = (B_0^2 + \varepsilon_2^2)^{1/2} < B,$$
$$\mu_1 = \left[\frac{(\gamma R_0/R_\varepsilon)^2 - 1}{\gamma^2 - 1}\right]^{1/2}, \quad \mu_2 = \left[\frac{(\gamma R_0/R_\varepsilon')^2 - 1}{\gamma^2 - 1}\right]^{1/2}. \tag{36}$$

The bounds (35) have a purely geometric nature: they are angles which characterize the intersection of the ellipsoid (34) with spheres of radii R_ε or R_ε'. The quantities μ_1 and μ_2 depend on the transferred energy ε, and on the boundary regions they reduce to zero or one. For example, according to (29), (30), μ_2 reduces to 1 as $|\varepsilon| \to B$ (region V'). This is important for the reason that in region V' the intercenter hopping of SP at large polar angles relative to the dislocation axis does not contribute to (33), because for $|\mu| < \mu_2$ the region of integration over R' disappears.

Each region of transferred energy corresponds to a region of hopping lengths; therefore, by calculating the integral over r' in (33) we obtain the exact expression (30), whose explicit form will depend on the specific region determined by (35). Here all the remarks in Sec. 4.1 are applicable concerning the relations (27), (30), (31) (Fig. 2).

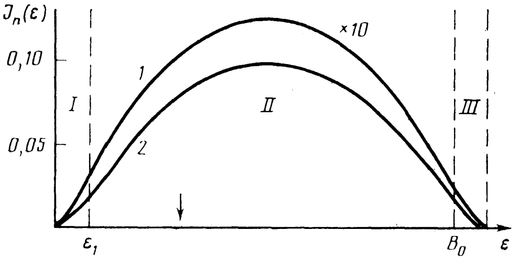

FIG. 2. Results of computer calculations of the integral (27) as a function of the energy ε transferred during hopping: *1*—$n = 0$, *2*—$n = 2$. The arrow indicates the upper limit on the transferred energy ($\hbar\omega_0$). In an anisotropic DBB system the boundaries between regions (I)–(III) are smeared out [see (35)], forming the transition regions (II′)–(IV′) from the three-dimensional regime to the one-dimensional regime of correlated DBB electron diffusion.

4.3. Change in effective dimensionality of the spin-correlated transport caused by thermalization of carriers in a narrow band

The importance of the $|\varepsilon|$-dependent angular bounds which appear in (35) clearly manifests itself as a change in the dimensionality of the thermally-activated transport of SP in the narrow-band DBB system during thermalization. In practice, as we showed in our discussion of the kinetic equation (22), in addition to the bounds on the value of the energy transferred during hopping, there exist the overall bounds (24), according to which the energy E of a carrier in a narrow band for $E < \hbar\omega_0$ is an upper bound on the transferred energy. Hence, in agreement with (35), the characteristic length for adiabatic hopping and its angular dependence are determined by one of the regions (I′)–(V′) as a function of the magnitude of the carrier energy E. In the case investigated in Sec. 4.2 of a system of oriented dislocations, regions (I′) and (II′) correspond to the regime of three-dimensional diffusion, while regions (IV′), (V′) correspond to one-dimensional diffusion; region (III′) is a transitional region from one-dimensional to three-dimensional diffusion as $|\varepsilon|$ (or E) decreases. Drawing this conclusion allows us to analyze the integral (33) in the most important and broadest region (III′), which overlaps region (II); see (28) and Fig. 2. The effective dimension of the diffusion is determined by the size of the angular integration region giving the principal contribution to the integral (33). In region (III′) we can use relation (31) for the radial integral, if in the latter we replace the radius R_0 by $R_0(\mu)$ from (34). Then the integral of interest is proportional to the following expression:

$$J_n'(\varepsilon) \propto \int_{-1}^{1} d\mu \left[\frac{R_0(\mu)}{a_1}\right]^n \exp\left[-\frac{2R_0(\mu)}{a_1}\right]. \tag{37}$$

In the case of an anisotropic system ($\gamma \gg 1$), the main angular dependence is introduced into the integral (37) by the exponential factor, compared to which the powers of $R_0(\mu)$ can be treated as slowly-varying functions. Then (37) can be written schematically in the form ($\alpha = (\gamma^2 - 1)^{-1} \ll 1$):

$$J_n'(\varepsilon) \propto \int_0^1 d\mu \exp\left[-\frac{\lambda}{(\mu^2 + \alpha^2)^{1/2}}\right] \approx \frac{e^{-\lambda}}{\lambda}, \quad \lambda = \alpha^{1/2}\gamma\frac{2R_0}{a_1}. \tag{38}$$

It is easy to see that the required region of polar angles giving the main contribution to the integral (38) is determined by the inequality

$$\mu^* = \frac{\lambda}{\lambda + 1} < |\mu| \leqslant 1, \tag{39}$$

i.e., the interior of a cone in which the hopping occurs principally in region (III′); the larger λ, the narrower this cone. Thus, one-dimensional diffusion will dominate in the transition region (III′), because the angles with $|\mu| \approx 1$ correspond to motion along the polar axis in the anisotropic system.

The tendency for the effective dimensionality to change is clearly apparent in Fig. 2, if we take into account the bounds (24): the total range of variation of the average energy $\langle E \rangle$ of carriers in a narrow band is divided into three subregions with different effective diffusion dimensions. The assertion that this change in dimensionality takes place is quite general, and is applicable not only to three-dimensional but also to two-dimensional systems. In the latter case, relations (35), (36) preserve their form, while the only change in the integral (33) is in the power n, which has no effect on the results (38), (39).

Let us estimate the characteristics of the spin-correlated transport of S- and T-centers along the broken bonds. For an anisotropic system of parallel dislocations with a surface density $\Delta = 10^9$ cm^{-2} generated in plastically deformed silicon, we have the following numerical parameters: $a_1 = a_2 = a = 1$ Å, $R_0 \approx b_1 = a = 5$ Å, $b_2 = \Delta^{-1/2} = 3\cdot 10^{-5}$ cm, $\gamma = 600$, $\alpha^{1/2}\gamma = 1$, $\lambda = 10$, and $\mu^* = 0.9$. Hence, according to (39), the diffusion is quasi-one-dimensional for almost all $|\varepsilon|$, with the exception of the region of very low temperatures ($k_B T \langle \varepsilon_1$). For the case of a one-dimensional chain ($d = 1$), when the Debye energy is small enough that $\hbar\omega_0 \langle B_0$ in the neighborhood of the dislocation,[24] the mean hopping time τ can be cast in the form

$$\frac{1}{\tau} = \frac{1}{2\pi}\left(\frac{a}{a_0}\right)^2 \frac{\Xi^2 I_0{}^2 e^{-\lambda}}{\rho v_s{}^5 \hbar^4 B_0} \int_0^{\hbar\omega_D} d\varepsilon\, \varepsilon\,[2\mathscr{N}(\varepsilon) + 1]. \tag{40}$$

If the Huang-Rhys factor (11) (i.e., the optimum number of phonons for the multiphonon transition) for spin-correlated hopping SP, e.g., for a T-center, is taken to be $\overline{N} = 6$, then the corresponding tunneling factor in (12) is found to be $K_0 = 2.5\cdot 10^{-3}$, $\varepsilon_1 = 2|I_0|\exp(-\lambda/2) = 5\cdot 10^{-4}$ eV. For values of the parameters typical of silicon ($\Xi = 10$ eV, $\rho = 2.42$ gm$\cdot$cm^{-3}, $v_s = 3.77\cdot 10^5$ cm/sec, $B_0 \approx B = 0.06$ eV, $\hbar\omega_0 = 50$ K, $T = 77$ K), Eq. (40) yields for τ an estimated value of $5\cdot 10^{-11}$ sec, which is in good agreement with the observed value.[5]

The diffusion coefficient of thermalized carriers located at the bottom of the narrow band decreases by roughly two orders of magnitude compared to the estimated $D_\tau = 5\cdot 10^{-5}$ cm^2/sec which follows from the data presented above. The decrease is proportional to the band energy E of a carrier [$E < \hbar\omega_0$ (24)]. The average energy lost by a T-center in one intercenter hop amounts to roughly $\hbar\omega_0$; therefore a T-center emits on the average about ten DA-phonons in the course of thermalization. Consequently, the thermalization time is two orders of magnitude smaller than the spin relaxation time for the unpaired background DBB electrons, i.e., $\tau = 10^{-5}$ sec.[8]

Depending on the temperature and physical conditions, the initial state of the DBB chain can include magnetic orderings of para-, ferro-, and antiferromagnetic type.[5,25] Then either the ξ_j are realizations of a random quantity with values 0 and 1, or all $\xi_j = 1$, or the values 0 and 1 alternate along the chain [see (12)]. The latter case is equivalent to doubling the period of the chain of spin-allowed sites. The dependence of the diffusion coefficient for polarized T-centers with $M = \pm 1$ on the spin state of the DBB system for the above three types of magnetic ordering, respectively, can be schematically represented in the form of the ratio

$${}^1/_4(1+P)^2 : 1 : e^{-\lambda}, \tag{41}$$

where P is the spin polarization of the DBB background electrons in the paramagnetic phase. For $P = 0$ the coefficient D_τ for the paramagnetic chain is four orders of magnitude smaller than for the ferromagnetic chain. Because exp $(-\lambda) = 4.5\cdot 10^{-5}$, the diffusion coefficient of a polarized T-center decreases by the same amount in the antiferromagnetic chain as compared to the ferromagnetic chain. The latter estimate demonstrates the important role of magnetization of the background DBB electrons in the transport of polarized T-centers (Sec. 5.2).

5. EFFECT OF MAGNETIZATION OF THE DBB ON THE DIFFUSION OF POLARIZED *T*-CENTERS AND THE OPTICAL POLARIZATION OF NUCLEAR MOMENTS

5.1. Effective residence time of a *T*-center on a given DBB

There are effects associated with populating the dislocatin chains not included in the kinetic equation (22) which can hinder the change in diffusion dimensionality in the course of thermalization. For example, the electrostatic fields of the S-centers on the chains block the diffusion of T-centers at the ends of segments of finite length, which hinders the transition to the three-dimensional diffusion regime. Such processes increase the effective residence time t_{eff} of a diffusing polarized T-center at a given DBB, thereby enhancing the effect of magnetization of the background electrons of the DBB.

In order to calculate t_{eff} as a function of the average length L_s of a segment of dislocation chain on which diffusion is blocked, we introduce the auxiliary quantity ($x_\pm = x \pm a_0/2$)

$$t_{\text{eff}} = \int_0^\infty \frac{dt}{(4\pi D_T t)^{1/2}} \int_{x_-}^{x_+} dx' \exp\left(-\frac{x'^2}{4D_T t} - \frac{t}{\tau_T}\right) \tag{42}$$

which is the residence time of a T-center on a site located at a distance x from the coordinate origin of the one-dimensional DBB chain when the T-center "starts off" from this origin at $t = 0$; D_τ is the average diffusion coefficient of a T-center (Sec. 4.3), and τ_T is the mean lifetime of a T-center. It is obvious that the summation (42) over all sites of the chain gives τ_T. The double integral (42) can be cast in the form

$$t_{\text{eff}} \approx \frac{\tau_T}{2\pi^{1/2}} \int_{u_-}^{u_+} du\, \Gamma\left(-\frac{1}{2}, u\right), \qquad u_\pm = \frac{x_\pm{}^2}{4D_T\tau_T}, \tag{43}$$

where $\Gamma(-\frac{1}{2}, u)$ is the incomplete gamma-function. Using the asymptotic properties of the latter[26] and taking into account that the characteristic scale of variation of the (42) is the diffusion length of a T-center $l_\tau = (D_T\tau_T)^{\frac{1}{2}} \gg a_0$, we obtain for (43) the following estimate:

$$t_{\text{eff}} = \begin{cases} (\tau_T\tau)^{1/2}, & |x| < l_T, \\ 0, & |x| > l_T, \end{cases} \tag{44}$$

where $\tau = a_0{}^2/D_T$, (40).

Now, along with (44) it is necessary to include the finite length of the segments L_s. It is obvious that for $L_s > l_T$ the character of the diffusion does not change, and the required effective residence time t_{eff} for a T-center on a given DBB averaged over sites of the segment equals $(\tau_T\tau)^{\frac{1}{2}}$, i.e., (44). In the opposite limit $l_\tau > L_s$ the time t_{eff} increases in proportion to the number of returns l_τ/L_s because of the "walls" which bound the segment; therefore we eventually find that

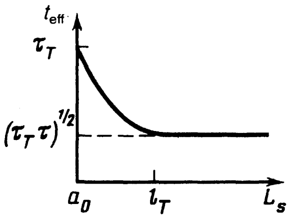

FIG. 3. Dependence of the effective residence time t_{eff} of a diffusing nonequilibrium T-center at a given DBB on the mean length L_s of a segment of a dislocation chain.

$$t_{\text{eff}}=\begin{cases}\tau_T(a_0/L_s), & L_s<l_T,\\ (\tau_T\tau)^{1/2}, & L_s>l_T.\end{cases} \tag{45}$$

The function (45) shown in Fig. 3 was observed by the OPNM method in plastically deformed silicon, taking the form of a dependence of the degree of occupation of the DBB by equilibrium electrons from shallow donors.[5]

We can show that the balance of spin polarization P of the background electrons of the DBB interacting with polarized T-centers according to the Van Vleck mechanism has the form

$$\dot{P}=-w_S(P-P_0)+w_f[P_T-P(1-N_0)], \tag{46}$$

where P_0 is the equilibrium polarization of the background electrons, P_T and N_0 are the spin polarization and relative occupation of the $M=0$ state of the T-centers, w_f and w_s are the spin-flip probabilities of a background electron due to interaction with a T-center and due to other spin-spin interactions in the system respectively ($w_f \gg w_s$). The case $N_0=0$, $T_T\neq 0$ corresponds to completely polarized T-centers, while the case $N_0=1$ ($P_T=0$) corresponds to completely unpolarized T-centers. For $N_0=1$, the T-centers are found to have no magnetizing effect on the background electrons of the DBB, because the occupation of their polarized states ($M=\pm 1$) equals zero. For $N_0=0$, $P_T=0$, the polarization of the background electrons reduces to a value smaller than the equilibrium polarization P_0. Hence, the factor $1-N_0$ in (46) describes a weakening of the polarizing effect of the T-centers with increasing N_0. In view of (45), the solution of Eq. (46) averaged over motion of the T-centers at the ends of a dislocation segment of given length L_s has the form

$$P_D=P_0+(P_\Phi-P_0)[1-\exp(-t_{\text{eff}}/\tau_2)], \tag{47}$$

$$1/\tau_2=w_S+w_f(1-N_0),\quad P_\Phi\approx P_T/(1-N_0),$$

where τ_2 is the effective spin-spin relaxation time of an individual DBB, and P_Φ is the maximum attainable value of polarization of the background electrons.

5.2. Optical polarization of nuclear moments under conditions of polarization and magnetic ordering of broken bonds

In silicon with edge dislocations OPNM arises because of hyperfine interaction of the ^{29}Si with polarized T-centers formed by trapping of photoexcited electrons at a DBB.[5,6] In weak magnetic fields the background electrons of the DBB which are polarized as a result of spin-correlated transport of T-centers along the broken bonds[5,10,11] give a contribution to OPNM and to the nuclear spin-lattice relaxation (Sec. 5.1). In order to investigate the influence of the effective correlation length (see the end of Sec. 2) and the magnetically-ordered broken bonds on the process of spin-correlated transport, in this paper we have studied the OPNM in plastically-deformed p-type silicon [$N(B)=10^{13}$ cm^{-3}]. The degree of deformation of the samples under uniaxial compression ($T=700$ °C) comes to $\varepsilon=5.1\%$ ($\Delta=1.2\cdot10^9$ cm^{-2}), the concentration of broken bonds $N_{\text{DBB}}=5.2\cdot10^{16}$ cm^{-3}. The presence of quasi-one-dimensional chains is monitored by the EPR method.[3,23]

The OPNM experimental method is described in detail in Refs. 5.17,28. We will dwell only briefly on the basic aspects: samples of plastically-deformed silicon are illuminated in a magnetic field with unpolarized light from a 200 W filament lamp. In the course of our investigation we varied the light pump intensity, the value of the external magnetic field (0.5 Oe–5 kOe) and the sample temperature (8–77 K). In order to measure the degree of OPNM P_n, the samples were transferred after illumination to a NMR radiospectrometer magnet, where the magnetization of ^{29}Si nuclei induced by the optical pumping was recorded. The magnitude of P_n is determined by measuring the amplitude of the NMR signal from the ^{29}Si nuclei; the direction of the nuclear magnetization relative to the external magnetic field is fixed by the phase of the NMR signal.

In the process of optical pumping the samples of plastically-deformed silicon, photoexcited electrons from the conduction band are selectively trapped on the magnetic sublevels of the triplet DBB states, as a result of which polarized T-centers are formed which interact with nearby ^{29}Si.[5,27,28] The nuclear magnetism which arises as a result of the hyperfine interaction is propagated throughout the entire volume of the crystal by means of nuclear spin diffusion, which is reflected in the kinetic dependences of P_n. The polarized T-centers, because of Hund's- rule interactions, can also orient the electrons of the dislocation chains in the course of spin-correlated hopping, which in turn induces a polarization of the ^{29}Si with subsequent spin diffusion in weak magnetic fields.[5,27,28] From the experimental kinetic dependences $P_n=P_{nm}[1-\exp(-t/T_1)]$[27,28], where P_{nm} is the limiting degree of polarization established in the volume of the crystal, and T_1 is the nuclear spin-lattice relaxation time taking into account spin diffusion, the characteristics of OPNM are determined as functions of pump light intensity, magnitude of the external magnetic field, and temperature (Figs. 4–6).

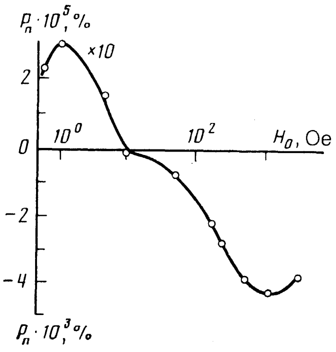

FIG. 4. Dependence of the degree of OPNM on the magnitude of the magnetic field in unannealed single-crystal p-type silicon plastically-deformed at 700 K by using uniaxial compression; $\varepsilon=5.1\%$.

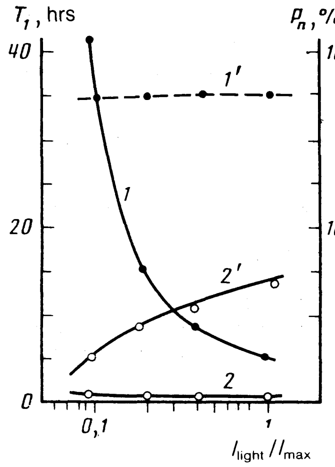

FIG. 5. Dependence of the nuclear spin-lattice relaxation time T_1 (curves *1* and *2*) and the degree of OPNM (curves *1'* and *2'*) on the pump light intensity $I_{\rm light}$ in plastically-deformed *p*-type silicon: *1,1'*—$H_0 = 5$ kOe; *2,2'*—1 Oe.

Our investigations showed that the contact interaction dominates in the hyperfine interaction of a *T*-center with ^{29}Si nuclei, while the polarized segments of DBB chains induce OPNM in weak magnetic fields because of dipole-dipole interactions (Fig. 4). The behavior of P_n is described by well-known functions[5,27,28]:

(a) In the region of strong magnetic fields,

$$P_n=\xi P_T, \qquad P_T=P_m\frac{\tau_{ST}}{\tau_{ST}+\tau_T}, \tag{48}$$

where ξ is an indicator of the relative contribution to the OPNM of the contact and dipole-dipole hyperfine interactions ($\xi<0$ in the case where the contact interaction dominates[27,28]); P_m is the maximum degree of polarization corresponding to the region of forbidden crossing of the magnetic sublevels of the triplet center[9]; $\tau_{\rm ST}$ is the spin-lattice relaxation time of *T*-centers.

(b) In the region of strong magnetic fields

$$P_n=\xi P_D=\xi P_T[1-\exp(-t_{\rm eff}/\tau_2)], \tag{49}$$

were P_D is defined in Eq. (47) ($N_0\approx 0$, $P_T\gg P_0$), $\xi>0$.

The degree of OPNM does not depend on the pump light intensity $I_{\rm light}$ (Fig. 5), because P_T is practically constant as a function of the distance L_s between nonequilibrium *S*-centers, which is limited by the motion of *T*-centers along the DBB chains.[5,6] At the same time, T_1 increases as the pump light intensity decreases (Fig. 5), because under these conditions the concentration of *T*-centers corresponding to the OPNM is decreasing: $1/T_1\propto N_T$. In weak magnetic fields T_1 is practically independent of $I_{\rm light}$ (Fig. 5), because in this case the OPNM and nuclear spin-lattice relaxation are determined by the DBB concentration: $1/T_1\propto N_{\rm DBB}$. The decrease in P_n as $I_{\rm light}$ falls off in weak magnetic fields (Fig. 5, curve 2') attests to the important role of $t_{\rm eff}$ in the process of polarization of DBB during the spin-correlated transport [see (47)]. Under these conditions, the distance L_s between *S*-centers decreasees, i.e., the mean length of a segment of the DBB chain which is polarized during spin-correlated transport of *T*-centers increases; as a consequence, $t_{\rm eff}$ decreases (Fig. 3), which gives rise to a decrease in P_D, (45), (47). Some of the increase of P_n as the temperature decreases is caused by the increase in $\tau_{\rm ST}$ [Fig. 6; see (48)]. However, since the samples under study had significant dislocation densities ($\Delta\approx 10^9$ cm^{-2}, $\tau_T\propto\Delta^{-1}$) and were close to optimal from the standpoint of obtaining a high degree of OPNM ($\tau_{\rm ST}\approx\tau_T\approx 10^{-8}$ sec at $T=77$ K), the growth in $\tau_{\rm ST}$ as the temperature is lowered is only weakly reflected in the value of P_n.

Let us examine the effect of decreasing T_1 as the temperature decreases (Fig. 6b) under conditions where the decisive contribution to the nuclear spin-lattice relaxation is from the DBB chains. The rate of nuclear relaxation in this case is described by the expression

$$\frac{1}{T_1}=2\pi N_{\rm DBB}\int_\delta^\infty\frac{r\,dr}{T_1(r)}, \tag{50}$$

where δ is the diffusion radius of a nuclear spin[27,28]; δ is determined from the following relation: $1/T_1=(\delta)\,D_s/a^2$ ($D_s=2.4\cdot 10^{-14}$ cm^2 sec^{-1} is the spin diffusion coefficient for a ^{29}Si nucleus in silicon; $a=6.5$ Å is the mean distance between ^{29}Si nuclei). The rate of local nuclear spin-lattice relaxation $1/T_1(r)$ is proportional to the square of the total spin of the dislocation segment $|\mathbf{I}|^2$ (Refs. 5,10), which grows as the temperature decreases because of magnetic ordering of the DBB through *T*-center motion along the chain. The quantity $|\mathbf{I}|$ depends on the effective correlation length R_c (see the end of Sec. 2): $|\mathbf{I}|=(R_c/a_0)P_D$; $R_c=(D_T\tau_1)^{\frac{1}{2}}$ [$D_T=5\cdot 10^{-5}$ cm^2 sec^{-1} is the diffusion coefficient of a *T*-center[5]; see also the estimate based on Eq. (40)]. The spin-lattice relaxation time for DBB electrons (τ_1) grows as the temperature decreases,[2,3] which leads to a growth of $|\mathbf{I}|$ and correspondingly of the probability (50). The calculated dependence of T_1 on T, (50), taking into account the parameters of the samples under study, are in good agreement with the experimental results [Fig. 6(b)]. It should be noted that the indirect exchange depends weakly on the distance

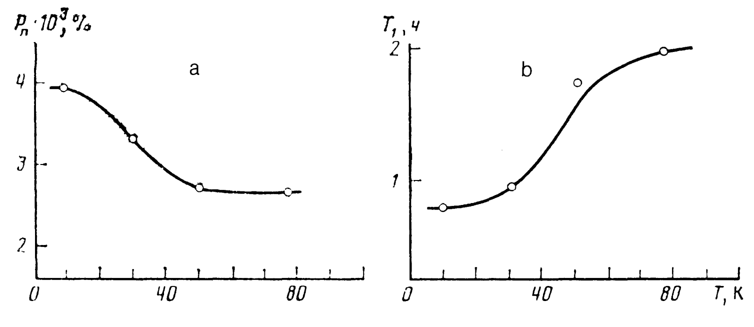

FIG. 6. Dependence of the degree of OPNM (a) and time T_1 (b) on temperature for plastically-deformed *p*-type silicon. The continuous curves are the calculated dependences.

between DBB in an ordered region of size R_c by virtue of the diffusive character of the T-center motion, from which follows the estimate of $|\mathbf{I}|$ presented above. An estimate of the DBB energy in the magnetically-ordered region, based on the self-consistent field approximation and the competition between indirect exchange via nonequilibrium T-centers and spin-Peierls dimerization, shows that the system under study becomes stable for $T < 50$–70 K. Hence, the decrease in T_1 as the temperature decreases [Fig. 6(b)] is a direct proof of the appearance of magnetic ordering in the DBB system via motion of T-centers within it.

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[1)] The Hamiltonian for an isolated DBB was studied in Ref. 6.

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[1] Yu. A. Osip'yan, J. de Phys. Colloq. **44**, C4-103 (1983).
[2] V. A. Grazhulis, V. V. Kveder, and V. Yu. Mukhina, Phys. Status Solidi (a) **43**, 407 (1977).
[3] V. A. Grazhulis, V. V. Kveder, and V. Yu. Mukhina, Phys. Status Solidi (a) **44**, 107 (1977).
[4] V. A. Grazhulis, V. V. Kveder, and Yu. A. Osip'yan, Phys. Status Solidi (b) **103**, 519 (1981).
[5] N. T. Bagraev and L. S. Vlasenko, Zh. Eksp. Teor. Fiz. **83**, 2186 [Sov. Phys. JETP **56**, 1266 (1983)].
[6] N. T. Bagraev, A. I. Gusarov, and V. A. Mashkov, Zh. Eksp. Teor. Fiz. **92**, 968 (1987) [Sov. Phys. JETP **65**, 548 (1987)].
[7] V. V. Kveder, Yu. A. Osipyan, W. Schröter, and G. Zoth, Phys. Status Solidi (a) **72**, 701 (1982).
[8] V. V. Kveder, Yu. A. Osipyan, and A. I. Shalynin, Zh. Eksp. Teor. Fiz. **83**, 699 (1982) [Sov. Phys. JETP **56**, 389 (1983)].
[9] L. S. Vlasenko, Izv. Akad. Nauk SSSR, Ser. Fiz. **46**, 469 (1982).
[10] N. T. Bagraev, L. S. Vlasenko, V. A. Mashkov, and V. A. Khramtsov, Fiz. Tverd. Tela (Leningrad) **28**, 634 (1986) [Sov. Phys. Solid State **28**, 358 (1986)].
[11] N. T. Bagraev, L. S. Vlasenko, and V. A. Mashkov, Fiz. Tverd. Tela (Leningrad) **28**, 1190 (1986) [Sov. Phys. Solid State **28**, 667 (1986)].
[12] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).
[13] P. W. Anderson, Phys. Rev. Lett. **34**, 953 (1975).
[14] N. T. Bagraev and V. A. Mashkov, Solid State Commun. **65**, 1111 (1988).
[15] T. Holstein, Ann. Phys. (USA) **8**, 343 (1959).
[16] *Polyarony* (Polarons), Yu. A. Firsov, ed., Nauka, Moscow, 1975.
[17] V. A. Kovarskiĭ, I. A. Chaikovskiĭ, and E. P. Sinyavskiĭ, Fiz. Tverd. Tela (Leningrad) **6**, 2131 (1964) [Sov. Phys. Solid State **6**, 1679 (1964)].
[18] A. Miller and E. Abrahams, Phys. Rev. **120**, 745 (1960).
[19] B. I. Shklovskiĭ and A. L. Efros, *Elektronnye Svoistva Legirovannykh Poluprovodnikov* (*Electronic Properties of Doped Semiconductors*), Nauka, Moscow, 1979.
[20] N. Mott and E. Davis, *Elektronnye Protsessy v Nekristalicheskykh Veshchestvakh* (*Electronic Processes in Non-crystalline Materials*). Mir, Moscow, 1982 (Oxford U. Press, 1971).
[21] B. I. Shklovskiĭ and A. L. Efros, Zh. Eksp. Teor. Fiz. **81**, 406 (1981) [Sov. Phys. JETP **54**, 218 (1981)].
[22] A. A. Gogolin, V. I. Mel'nikov, and E. I. Rashba, Zh. Eksp. Teor. Fiz. **69**, 327 (1975) [Sov. Phys. JETP **42**, 168 (1975)].
[23] V. A. Grazhulis, V. V. Kveder, and Yu. A. Osip'yan, Phys. Lett. A **66**, 398 (1978).
[24] V. M. Vinokur and V. Ya. Kravchenko, Pis'ma Zh. Eksp. Teor. Fiz. **29**, 626 (1979) [JETP Lett. **29**, 572 (1979)].
[25] S. V. Broude, V. A. Grazhulis, V. V. Kveder, and Yu. A. Osip'yan, Zh. Eksp. Teor. Fiz. **66**, 1469 (1974) [Sov. Phys. JETP **39**, 721 (1974)].
[26] I. S. Gradshtein and I. M. Ryzhik, *Tablitsy Integralov, Summ, Ryadov i Proizvedenii* (*Tables of Integrals, Sums, Series and Products*, Academic Press, New York, 1965). Nauka, Moscow, 1971.
[27] N. T. Bagraev and L. S. Vlasenko, Zh. Eksp. Teor. Fiz. **75**, 1743 (1978) [Sov. Phys. JETP **48**, 878 (1978)].
[28] N. T. Bagraev and L. S. Vlasenko, Fiz. Tverd. Tela (Leningrad) **21**, 120 (1979) [Sov. Phys. Solid State **21**, 70 (1979)].

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