Multiphonon ionization of deep point centers in the field of a charged dislocation

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The probability for multiphonon ionization of a deep negative ion in the field of a charged dislocation is calculated in the quasiclassical approximation. The analytical dependence of the probability on the electron-phonon coupling constant, temperature, and charge per unit dislocation length is derived. The dependence of the ionization probability on the distance between the center and the dislocation is plotted for ZnSe.

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1. INTRODUCTION

When a crystal is plastically deformed, a point center can appear in the space-charge region surrounding a charged dislocation. Under these conditions a tunneling transition of electrons from the center into the conduction band of the semiconductor is possible. The electrostatic potential of the dislocation in cylindrical coordinates (r, θ, z) with the z axis taken along the dislocation has the form[1]

$$e\varphi(r) = U_0 \ln(\rho/r), \quad r \leqslant \rho, \tag{1}$$

where $U_0 = 2e^2 f(T)/\varepsilon_0 a$, ε_0 is the dielectric constant, a is the distance between atoms on the dislocation, ρ is the screening radius, and $f(T)$ is the temperature dependent filling coefficient of the dislocation by electrons.

It is well known that field-induced ionization of a deep center can precede the electron activation caused, in the range of sufficiently high temperatures, by the electron-phonon interaction. Such an inelastic process in general has a multiquantum character. Multiphonon ionization of deep centers in a uniform electric field was studied by Kudzhmauskas[2] and Dalidchik.[3] It was shown in these papers that in a strong electric field, when tunneling processes are instantaneous in comparison to the vibrational subsystem, the electron-phonon interaction is negligible. However in weak fields, when the tunneling is slow, the dynamical coupling of the electron with the lattice is quite substantial. In connection with this, we note that because of the weak nonuniformity of the electrostatic potential of the dislocation (resulting from the symmetry of the problem), it is necessary in principle even in the case of strong fields of order 10^6 V/cm, to take into account the electron-phonon interaction in the ionization of a deep center.

In our paper, we have used the usual theory of multiphonon transitions developed by Perlin[4] and Rickayzen.[5] We limit ourselves to the study of the interaction of electrons with acoustic phonons, the spectrum of which is assumed to be of the Debye type up to a limiting wave number q_m which is connected with the elementary-cell volume V_0 by the relation $q_m^3 V_0 = 6\pi^2$. For the interaction we use the usual isotropic deformation potential:

$$H_{int} = \frac{iE_c}{N^{1/2}} \sum_{\mathbf{q}} qF(q)\,(b_{\mathbf{q}} - b_{-\mathbf{q}}^{+})\, e^{i\mathbf{qr}}. \tag{2}$$

Here $F(q) = (\hbar/2M\omega_q)^{1/2}$, $\mathbf{r}$ is the radius vector, E_c is the deformation-potential constant, N is the number of elementary cells in the main volume, M is the mass of an elementary cell, b_q^+ and b_q are the phonon creation and annihilation operators, and ω_q is the frequency of a phonon with wavevector $\mathbf{q}$. Allowance for the local oscillations coupled to the center, the anharmonicity, the frequency effect,[4] and also for degeneracy and for a more realistic dispersion law for the band electrons, are all outside of the scope of this paper and would require special treatment.

2. FORMULATION OF THE PROBLEM. TUNNELING

Being interested in the ionization of a deep point center constituting a negative ion, we approximate the neutral atomic residue of the ion by a potential of zero radius.[6] Then the wave function of an electron localized on a center (state m) which is a distance r_0 from the axis of the dislocation in the $z = 0$ plane has the following form in cylindrical coordinates:

$$\psi_m = \left(\frac{\varkappa}{2\pi}\right)^{1/2} \frac{\exp\{-\varkappa[(r-r_0)^2+z^2]^{1/2}\}}{[(r-r_0)^2+z^2]^{1/2}}, \tag{3}$$

where $\varkappa = (2mE_I^0/\hbar^2)^{1/2}$, and E_I^0 is the unperturbed ground-state energy.

As we noted earlier,[7] an edge dislocation in an electronic semiconductor leads to a one-dimensional band with the bottom E_D in the forbidden band. Ignoring transitions of the electron from a point center to the dislocation, we confine ourselves to distances $r_0 \gg \varkappa_D^{-1}$, where $\varkappa_D^{-1} = (\hbar^2/2mE_D)^{1/2}$ is the localization radius of an electron on the dislocation. Then the quasiclassical wave function of the band electron in the field of the dislocation [Eq. (1)] (state n), normalized to a cylinder of radius R and length L_z) is given by the expression:

$$\psi_n = \left(\frac{k}{4\pi RL_z}\right)^{1/2} \exp\left\{-\frac{(2mU_0)^{1/2}}{\hbar} r(E)\,\gamma\left[\frac{3}{2}; \ln\frac{r(E)}{r}\right]\right\} \frac{\exp(ik_z z)}{(|k(r)|r)^{1/2}}, r < r(E), \tag{4}$$

where $E = \hbar^2(k^2 + k_z^2)/2m$; k_z and k are the wavenumbers corresponding to motion of the electron along and transverse to the axis of the dislocation, respectively. $\gamma(n; x)$ is the incomplete gamma function,[8] and $r(E)$ is the turning point defined by the condition

$$k(r) = \frac{1}{\hbar}\{2m[E - e\varphi(r)]\}^{1/2} = 0. \tag{5}$$

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Here we consider s-ionization, and so we put the orbital angular momentum quantum number l equal to zero. We assume that the wave function of the localized state is not modified by the electric field of the dislocation. Then the action of the field reduces to a shift in the ground-state level E_I^0 due to the distortion of the band

$$E_I = E_I^0 - e\varphi(r_0). \tag{6}$$

In a sufficiently strong field such a shift can lead to an effective interaction of the impurity level E_I with the conduction band and therefore ensure tunneling transitions of the electron from the center into the band. However, in the case of interest to us the field is only weakly non-uniform, the transparency of the barrier turns out to be small, and the tunneling time is rather large. Preliminary activation of the electron, which shortens the tunneling path, is therefore advantageous. A possible activation channel is a multiphonon transition.

We will treat the interaction of the electrons with phonons in the adiabatic approximation. In the adiabatic approach, the probability of an n-phonon transition arises even in the first order of perturbation theory, while in the usual perturbation theory such a multiphonon transition is possible only in higher orders and has an extremely small probability.[4] We note that a band electron does not perturb the lattice, whereas a localized electron, following a transition into the band, causes a lattice polarization due to the finite displacements of the equilibrium positions of the phonon normal coordinates. This leads to the possibility of absorption of a large number of phonons by the electron in a single event, and its activation into the region of large energies. The probability of such a multiphonon field-induced ionization has the form[2,3]

$$W_{mn} = \int_{-\infty}^{\infty} w(\varepsilon) g(\varepsilon)\, d\varepsilon, \tag{7}$$

where

$$w(\varepsilon) = \frac{2\pi}{\hbar} \sum_{k, k_z} \left| \int d^3 r\, \psi_n^* \, e\varphi(r) \psi_m \right|^2 \delta(E + E_I - \varepsilon) \tag{8}$$

is the tunneling probability per unit time of an electron from the impurity level $E_I - \varepsilon$ into the conduction band without the participation of phonons, while

$$g(\varepsilon) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \exp\left\{ -\frac{i}{\hbar} \varepsilon t - \sum_q |A_q|^2 [i \sin \omega_q t + (2n_q + 1)(1 - \cos \omega_q t)] \right\} \tag{9}$$

is the probability of a multiphonon transition.[6] Here A_q is a dimensionless parameter characterizing the displacement of the normal coordinates of the phonons.

We find the probability $\omega(\varepsilon)$ of the purely electronic transition. For the calculation of the matrix element we use the integral representation

$$\frac{\exp\{-\varkappa[(r-r_0)^2 + z^2]^{1/2}\}}{[(r-r_0)^2 + z^2]^{1/2}} = \varkappa \int_1^{\infty} du\, e^{-\varkappa u |z|} J_0[\varkappa (r - r_0)(u^2 - 1)^{1/2}], \tag{10}$$

where $J_0(x)$ is a Bessel function of the first kind. Using Eqs. (3) and (4) for the wave functions, and carrying out successive integrations with respect to z and u, remembering that $k_z \ll \varkappa$, we easily find for the matrix element

$$M_{mn}(k, k_z) = \left(\frac{2k\varkappa}{RL_z}\right)^{1/2} U_0 \int_{r_0}^{\infty} dr \frac{r \ln(\rho/r)}{(|k(r)|r)^{1/2}} \times \exp\left\{ -\frac{(2mU_0)^{1/2}}{\hbar} r(E) \gamma\left[\frac{3}{2}; \ln\frac{r(E)}{r}\right] \right\} K_0[\varkappa(r - r_0)]. \tag{11}$$

where $K_0(x)$ is a Macdonald function. Putting $\varkappa r_0 \gg 1$ and noting that the principal contribution to the integral is made by a small region around the point $r = r_0$, we have after integration with respect to r

$$M_{mn}(k, k_z) = \left(\frac{2kr_0}{RL_z \varkappa |k(r_0)|}\right)^{1/2} e\varphi(r_0) \times \exp\left\{ -\frac{(2mU_0)^{1/2}}{\hbar} r(E) \gamma\left[\frac{3}{2}; \ln\frac{r(E)}{r_0}\right] \right\}. \tag{12}$$

Substituting the matrix element (12) into (8) and transforming, as usual, from sums over k and k_z to integrals, we obtain after integration with respect to k

$$w(\varepsilon) = \frac{E_I''}{\pi\hbar} \left(\frac{e\varphi(r_0)}{E_I''}\right)^2 \varkappa r_0 \int_{-\infty}^{\infty} dk_z \left(\frac{2mU_0}{\hbar^2} \ln\frac{r(k_z)}{r_0}\right)^{-1/2} \times \exp\left\{ -2\frac{(2mU_0)^{1/2}}{\hbar} r(k_z) \gamma\left[\frac{3}{2}; \ln\frac{r(k_z)}{r_0}\right] \right\}, \tag{13}$$

where

$$r(k_z) = r(\varepsilon) \exp(\hbar^2 k_z^2 / 2mU_0), \qquad r(\varepsilon) = \rho \exp[(E_I - \varepsilon)/U_0]. \tag{14}$$

It must be noted that the case of practical interest is when the external electric field is much weaker than the the characteristic atomic fields[9]

$$U_0 / r_0 \ll (2m)^{1/2} (E_I^0 - \varepsilon)^{3/2} / \hbar. \tag{15}$$

If this condition is satisfied, the decay of the ion occurs mainly along directions close to that of the electric field. Using (1), (6), (14), and also the properties of the incomplete gamma function, it is possible to show that when the inequality (15) is satisfied, the argument of the exponential in (13) is large. Therefore the integral with respect to k_z can be evaluated by the method of steepest descent. In order to do this, we need the extremum of the exponent. Since $\gamma(n; x)$ for $n \geqslant 0$ does not have any zeroes (except when $x = 0$), it is easy to see that the steepest-descent path corresponds to $k_z = 0$. Hence the final expression for $w(\varepsilon)$ takes the form

$$w(\varepsilon) = w_0(\varepsilon) \exp\left\{ -2\frac{(2mU_0)^{1/2}}{\hbar} r_0 \gamma\left[\frac{3}{2}; \frac{E_I^0 - \varepsilon}{U_0}\right] \right\} \exp\frac{(E_I^0 - \varepsilon)}{U_0}, \tag{16}$$

where

$$w_0(\varepsilon) = \frac{\varkappa r_0 E_I^0}{\pi\hbar} \left(\frac{e\varphi(r_0)}{E_I^0}\right)^2 \left\{ \frac{(2mU_0)^{1/2}}{\hbar} r_0 \frac{E_I^0 - \varepsilon}{U_0} \times \gamma\left[\frac{1}{2}; \frac{E_I^0 - \varepsilon}{U_0}\right] \exp\frac{(E_I^0 - \varepsilon)}{U_0} \right\}^{-1/2}. \tag{16a}$$

The exponential dependence of the tunneling path on the energy ε stems from the cylindrical symmetry of the problem and is due to the logarithmically weak nonuniformity of the charged dislocation field.

To conclude this section we note that the quasiclassical approximation is applicable when

$$\left| \frac{1}{k^2(r)} \frac{dk(r)}{dr} \right|_{r = r_0} \ll 1 \tag{17}$$

and this is equivalent to (15).

3. FIELD-INDUCED MULTIPHONON IONIZATION PROBABILITY

In Eq. (9) for the multiphonon ionization probability, the integral over t cannot in general be calculated. However, because the tunneling probability $w(\varepsilon)$ is a rapidly increasing function of ε, the main contribution to the integral occurs at small t. Expanding the exponential in powers of t and keeping terms of order t^2, we obtain for $g(\varepsilon)$ after elementary integration

$$g(\varepsilon)=\frac{1}{2\pi\hbar}\left(\frac{2\pi}{\sigma^2}\right)^{1/2}\exp\left[-\frac{(\varepsilon+\Delta)^2}{2\hbar^2\sigma^2}\right], \tag{18}$$

where

$$\Delta=\sum_q |A_q|^2\hbar\omega_q, \tag{19}$$

$$\sigma^2=\sum_q |A_q|^2\omega_q^2(2n_q+1), \tag{20}$$

$$A_q=(\hbar/2M\omega_q)^{1/2}a_q,\quad a_q=\frac{1}{N^{1/2}}\frac{iE_c}{\hbar s}\int d^3r|\psi_m|^2e^{iqr}. \tag{21}$$

Here s is the velocity of sound, and $n_q=[\exp(\hbar\omega_q/kT)-1]^{-1}$ are the phonon occupation numbers. Hence according to (7) the probability of a field induced multiphonon ionization reduces to an average of the electronic factor $w(\varepsilon)$ over the Gaussian distribution (18). This approximation of $g(\varepsilon)$ is correct when the condition

$$\sum_q |A_q|^2(\hbar\omega_q)^3\frac{\varepsilon+\Delta}{\hbar^4\sigma^4}\left|\frac{(\varepsilon+\Delta)^2}{6\hbar^2\sigma^2}-1\right|\ll 1 \tag{22}$$

is fulfilled. This condition is satisfied when the temperature is sufficiently high, and (or) the coupling of the localized carrier with the lattice is not small.[10]

We now calculate the integral over ε in (7), again using the method of steepest descent. Then the final expression for the ionization probability takes the form:

$$W=2\frac{\varkappa r_0}{\hbar}\left(\frac{e\varphi(r_0)}{E_I^0}\right)^2\frac{E_I^2}{\hbar\sigma}F(\varepsilon_n)\frac{\exp\{-f(\varepsilon_n)\}}{(|f''(\varepsilon_n)|)^{1/2}}, \tag{23}$$

where

$$F(\varepsilon)=\left\{\frac{(2mU_0)^{1/2}}{\hbar}r_0\frac{E_I^0-\varepsilon}{U_0}\gamma\left[\frac{1}{2};\frac{E_I^0-\varepsilon}{U_0}\right]\exp\frac{(E_I^0-\varepsilon)}{U_0}\right\}^{-1/2},$$
$$f(\varepsilon)=2\frac{(2mU_0)^{1/2}}{\hbar}r_0\gamma\left[\frac{3}{2};\frac{E_I^0-\varepsilon}{U_0}\right]\exp\frac{(E_I^0-\varepsilon)}{U_0}+\frac{(\varepsilon+\Delta)^2}{2\hbar^2\sigma^2}, \tag{24}$$

and the saddle point value of ε_n is determined by

$$Ae^x\gamma[1/2;\,x]=B-x, \tag{25}$$

in which

$$A\equiv\frac{(2mU_0)^{1/2}}{\hbar}\left(\frac{\hbar\sigma}{U_0}\right)^2r_0,\quad B\equiv\frac{E_I^0+\Delta}{U_0},\quad x\equiv\frac{E_I^0-\varepsilon_n}{U_0}>0. \tag{26}$$

In order to find an approximate analytical solution to (25) we first determine its coefficients. We use wave function (3) of the localized state

$$\psi_m=\left(\frac{\varkappa}{2\pi}\right)^{1/2}\frac{e^{-\varkappa r}}{r}$$

transformed to spherical coordinates with the origin at the negative ion. According to (21) the displacements of the normal coordinates of the phonons are then

$$a_q=\frac{2\varkappa}{N^{1/2}}\frac{iE_c}{\hbar\omega_q}\operatorname{arctg}\left(\frac{q}{2\varkappa}\right). \tag{27}$$

Substituting (27) in (19) and going over from a sum to an integral with respect to q, we have for the "heat release" Δ that characterizes the energy of the lattice polarization due to the activation of the electron

$$\Delta=\frac{3\pi^2}{2}\frac{m}{M}\left(\frac{E_c}{\hbar\omega_m}\right)^2E_I^0, \tag{28}$$

where we have used the condition $\hbar\omega_m\gg(8ms^2E_I^0)^{1/2}$. To find $\hbar^2\sigma^2$ we consider the two limiting cases of high and low temperatures.

1. $kT\gg\hbar\omega_m$—the classical limit. Expanding the exponential in n_q with respect to $\hbar\omega_q/kT$, we obtain after a simple integration

$$\hbar^2\sigma^2=2\Delta kT. \tag{29}$$

2. $(8ms^2E_I^0)^{1/2}\ll kT\ll\hbar\omega_m$—the quasiclassical limit. Since in the integral containing n_q only large values of q are significant, we use the asymptotic form of $\arctan(q/2\varkappa)$ and replace the upper limit of the integral by infinity. This corresponds to discarding terms of order $(\hbar\omega_m/kT)\exp(-\hbar\omega_q/kT)$. We then find

$$\hbar^2\sigma^2=\frac{\Delta\hbar\omega_m}{2}\left[1+\frac{2\pi^2}{3}\left(\frac{kT}{\hbar\omega_m}\right)^2\right]. \tag{30}$$

From (18), (29), and (30) it is seen that at high temperatures the multiphonon transition proceeds mainly via activated states located the intersections of the adiabatic potentials with activation energy $E^*=(\varepsilon+\Delta)^2/4\Delta$. At low temperatures the system perfers the classical tunneling transition between the electron-vibrational terms.

Returning now to equation (25), we obtain its approximate analytical solution. Assuming $x\ll 1$ it is easy to verify that the transcendental equation reduces to a simple quadratic equation with the root

$$x=A^2[(1-B/A^2)^{1/2}-1]^2. \tag{31}$$

The condition $x\ll 1$ corresponds to large distances r_0, where the strength of the dislocation field is small. For this tunneling the path is $r_T\ll r_0$. Physically the limiting case $x\ll 1$ is equivalent to the approximation of a uniform field[2,3] of strength U_0/r_0, since for a short sub-barrier tunneling path one may ignore the dependence on r_0. If r_0 is so large that $B/A^2\ll 1$ then for the saddle-point energy we easily obtain

$$\varepsilon_n=E_I^0-(B/2A)^2U_0. \tag{32}$$

From (32) it is clear that ε_m increases with distance of the point center from the dislocation, and therefore the

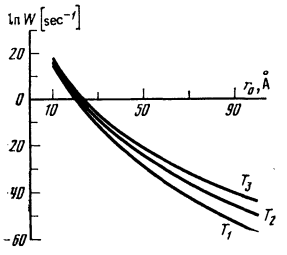

FIG. 1. Dependence of the ionization probability on r_0 for a center with $E_I^0=0.8$ eV at temperatures $T_1=300$ °K, $T_2=350$ °K, $T_3=400$ °K.

tunneling path drops off. Obviously beyond a certain critical value $r_{0\,cr}$, the quasiclassical treatment breaks down because the condition (17) is violated. The tendency for the tunneling path to increase as the center and the dislocation approach one another also takes place at small distances corresponding to $x \gtrsim 1$. However in this case an analytical solution to (25) cannot be obtained and numerical methods are necessary to find the saddle point energy.

4. NUMERICAL RESULTS

For the purpose of obtaining numerical values of the probability of ionization of a negative ion by the field of a dislocation we used the most typical values for the parameters of a II-VI semiconductor. The results of the calculation showed that at fixed r_0 the ionization probability is an increasing function of temperature. In particular, for ZnSe with $a=4\times10^{-8}$ cm, $m=0.17m_0$, $M=9.7\times10^{-22}$ g, $\hbar\omega_m=0.33$ eV, $\varepsilon_0=9.12$, $s=5\times10^5$ cm/sec (see Ref. 11), $E_I^0=0.8$ eV, $\rho=3\times10^{-6}$ cm, $E_c=11.5$ eV (see Ref. 12), and $f\sim0.5$, the dependence of $\ln W$ on r_0 for different temperatures is given in Fig. 1. The closeness of the curves corresponding to different temperatures reflects the nonlinearity in the temperature dependence of the saddle-point energy; this dependence is strongest at small distances.

Since in the calculation of the ionization probability of a deep center we assumed that all of the dislocations are independent and did not take into account possible overlaps of the electrostatic fields of different dislocations, the $\ln W(r_0)$ curves in the figure should be considered as lower limits.

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