Effect of electron-phonon interaction on the ionization of deep centers by a strong electric field

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(Submitted 4 July 1986)
Pis'ma Zh. Eksp. Teor. Fiz. **44**, No. 7, 334–336 (10 October 1986)

An expression is derived for the probability for the cold emission of an electron in the theory of multiphonon transitions. The interaction with local vibrations is taken into account.

In a strong electric field, the ionization of an impurity center occurs as a result of a tunneling of an electron from a bound state to a free state (Fig. 1). When there is an electron-phonon interaction, the ionization of a center should be accompanied by a change in the structure of the lattice near the center. Our purpose in the present letter is to show that this circumstance affects the probability for cold emission: In the argument of the tunneling exponential function, which determines the probability for ionization by a strong field, the thermal binding energy is replaced by a larger energy: an optical binding energy.

For simplicity, we assume that the lattice subsystem (the "nucleus") is described by a single configurational coordinate (a local vibration dominates the electron-phonon interaction). Figure 2 shows adiabatic terms for the motion of the "nucleus": U_1 corresponds to the bound state, and U_2 and U_ϵ correspond to the ionized center and to a free electron of energy ϵ (U_2 corresponds to $\epsilon = 0$; the scale for the energy of the emitted electron is shown in Fig. 1). The ionization is accompanied by a transition of the "nucleus" from term U_1 to U_ϵ. At low temperatures, this transition occurs through the tunneling of the "nucleus." The ionization probability is determined by a competition between the tunnel barrier for the "nucleus" and the electron: As $|\epsilon|$ increases (as U_ϵ decreases), the "nucleus" finds the transition easier, but the electron finds the tunneling more difficult. In a weak field, the optimum energy of the emitted electron is far lower than the thermal binding energy ϵ_T, and the characteristic term U_ϵ lies near U_2 (Ref. 1). As the electric field is intensified, the characteristic term U_ϵ descends to a lower position, and in the limit of strong fields the ionization probability

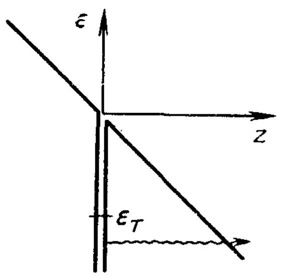

FIG. 1. Tunneling of an electron (↝) in a strong electric field.

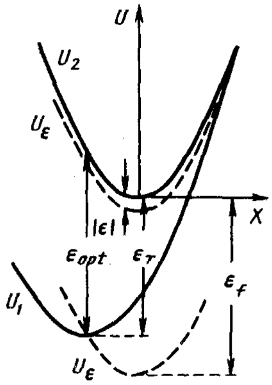

FIG. 2. Diagram of adiabatic terms for the motion of the "nucleus."

is determined by the most favorable conditions for the transition of the "nucleus." These conditions correspond to an arrangement of U_1 and U_ϵ such that they cross at the point of the minimum of U_1. As a result, the probability for ionization by a strong field F can be written with exponential accuracy as

$$W \sim \exp\left[-\frac{4}{3}\frac{\sqrt{2m}}{\hbar F}\epsilon_f^{3/2}\right], \tag{1}$$

where ϵ_f is greater than the thermal binding energy ϵ_T (Fig. 2). This effect is analogous to the familiar difference between the optical ($\epsilon_{\rm opt}$) and thermal binding energies; from Fig. 2 we see that the relation $\epsilon_f = \epsilon_{\rm opt}$ holds.

If the binding energy is comparable to the gap width E_g, a two-band spectrum must be taken into account in order to calculate the tunneling integral for the electron. In the Kane model we find expression (1), in which the "field binding energy" ϵ_f must be replaced by ϵ_f^*, defined by

$$\epsilon_f^{*3/2} = \frac{3}{8}E_g^{3/2}\{\arcsin\sqrt{u} - (1-2u)\sqrt{u(1-u)}\};\ u \equiv \frac{\epsilon_f}{E_g}. \tag{2}$$

Let us find the field and temperature correction to the exponential function for the probability for the cold emission of an electron in (1). In the case of a strong field, in which the bottom of the characteristic term U_ϵ lies near the bottom of U_1, the barrier for the "nucleus" is determined primarily by the term U_1. The probability for a transition of the "nucleus" can then be estimated as the probability for find the "nucleus" at the crossing of the terms for the case of an equilibrium distribution among the vibrational levels of the term U_1 (Ref. 2): $W_c \sim \exp[-2(\tilde{\epsilon}_1/\hbar\omega_1)\times {\rm th}(\hbar\omega_1/2k_BT)]$, where $\tilde{\epsilon}_1$ is the energy at which terms U_1 and U_ϵ cross reckoned from the bottom of U_1; and ω_1 is the frequency of the vibrations in the term U_1. The probability for the emission of an electron with an energy ϵ is proportional to the product of W_c and the electron tunneling probability:

$$W(\epsilon) \sim \exp\left[-2\frac{\tilde{\epsilon}_1}{\hbar\omega_1}\tanh\frac{\hbar\omega_1}{2k_BT}\right]\exp\left[-\frac{4}{3}\frac{\sqrt{2m}}{\hbar F}|\epsilon|^{3/2}\right]. \tag{3}$$

The term crossing energy $\tilde{\epsilon}_1$ is at a minimum, zero, at $|\epsilon| = \epsilon_f$, so that its relation with the energy of the emitted electron can be written as follows under the condition $\epsilon_f - |\epsilon| \ll \epsilon_f$:

$$\tilde{\epsilon}_1 = \frac{1}{b\epsilon_f} (\epsilon_f - |\epsilon|)^2, \tag{4}$$

where b is determined by the electron-phonon coupling constant.

The ionization probability W is equal to the sum of $W(\epsilon)$ over all states of the emitted electron. Using (4) and the method of steepest descent, we find the following expression for W:

$$W \sim e^{-\Phi_c}, \quad \Phi_c = \frac{4}{3} \frac{\sqrt{2m}}{\hbar F} \epsilon_f^{3/2} - b \frac{m\omega_1}{\hbar} \frac{\epsilon_f^2}{F^2} \coth \frac{\hbar\omega_1}{2k_B T} . \tag{5}$$

This expression describes the effect of the interaction of the electron with local vibrations of the "nucleus" on the ionization of the center of the strong electric field. If $k_B T < \hbar\omega_1$, it holds at $F > \sqrt{2m\epsilon_f}\omega_1$.

The relation between ϵ_f and ϵ_T and that between the constant b and the electron-phonon coupling constant are determined by the particular model used for the adiabatic terms. For example, if we assume that the adiabatic terms are identical parabolas (the Huang-Rys model[3]), we would have $\epsilon_f = \epsilon_T + S\hbar\omega_1$ and $b = 4S\hbar\omega_1/\epsilon$, where S is the Huang-Rys factor. Incorporating the Kane spectrum, we find expression (5), in which we need to make the replacement $\epsilon_f \to \epsilon_f^*$ in the first term for Φ_c and $b \to b^* = b(1 - \epsilon_f/E_g)$ in the second.

The coefficient of the exponential function in the ionization probability can be calculated in the model of a zero-radius potential, with the nonadiabaticity operator used as the perturbation which causes the transitions. As a result, we find

$$W = \frac{F}{2\sqrt{2m\epsilon_f}} e^{-\Phi_c}, \tag{6}$$

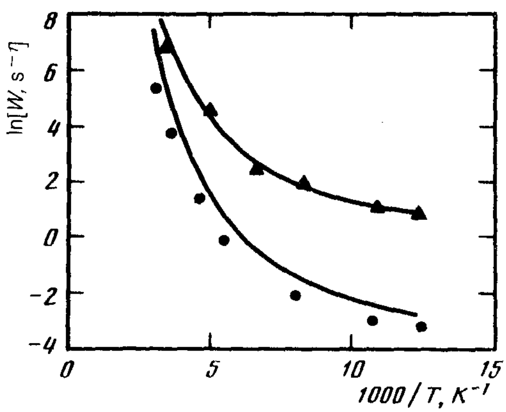

FIG. 3. Logarithm of the probability for the emission of electrons from the deep center EL2 in GaAs versus the reciprocal of the temperature for (▲) $F = 4\times10^5$ eV/cm and (●) $F = 3.5\times10^5$ eV/cm (Ref. 6). The curves are plots of expressions (6) and (5) for the parameter values found for the center in Ref. 7.

where the leading term in Φ_c is given by (5).

In deriving (6) we used the relation $S > 1$. At small values of S, at which the electron-phonon interaction can be ignored, expression (6) becomes the expression derived by Demkov and Drukarev[4] for the probability for cold emission.

Some previous theoretical papers[5,6] on multiphonon ionization of deep centers in a strong electric field gave expressions for W in a form requiring numerical calculations.

Figure 3 compares the expression found for W with the experimental data of Ref. 6 on the ejection of electrons from a deep level EL2 in GaAs in a strong field. The solid curves are drawn from expressions (6) and (5) for the parameter values $\epsilon_T = 0.73$ eV, $S = 5.5$, and $\hbar\omega_1 = 20$ meV, found in Ref. 7 through an analysis of the spectrum of photoluminescence from this level. It should be noted that expressions (6) and (5) not only correctly predict the thermal and field dependence of the ionization probability but also lead to the correct numerical value of W.

I wish to thank V. I. Perel' for constant interest and for assistance in this study.

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Translated by Dave Parsons