Thermoionization of deep centers in semiconductors in an electric field

V. Karpus and V. I. Perel'
A. F. Ioffe Physicotechnical Institute, Academy of Sciences of the USSR

(Submitted 5 October 1985)
Pis'ma Zh. Eksp. Teor. Fiz. **42**, No. 10, 403–405 (25 November 1985)

The expression for the dependence of the probability of thermalization on the external electric field is derived with exponential accuracy in terms of the theory of many-phonon transitions. An agreement with the experimental data on thermal ionization of deep impurities in silicon is obtained.

The effect of the electric field on the thermal ionization of impurity centers is usually linked with the Frenkel-Pool[1] effect. This effect, which involves the lowering of ionization energy by the electric field, is appreciable in the case of attractive Coulomb centers. The data obtained by capacitive spectroscopy—the principal method of studying thermal ionization—contradict the theory based on the Frenkel-Pool effect.[2] In the present letter we show that the experimental data are in agreement with the description of thermal ionization as a process of thermally stimulated tunneling of a vibrational system (a "nucleus") between two terms which correspond to a bound and a free state of an electron.[3] In an electric field an electron can be tunneled. As a result, the barrier for the tunneling of a "nucleus" is reduced and the probability of thermal ionization increases.

In a very simple model, which takes into account the interaction of an electron with only one type of local oscillations, the terms can be illustrated by a diagram in Fig. 1a, where x is the coordinate of the "nucleus," $U_1(x)$ and $U_2(x)$ are the potential

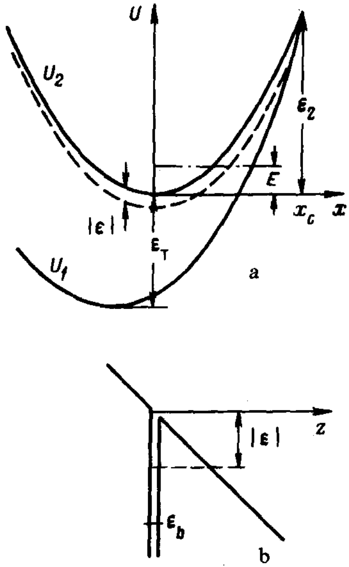

FIG. 1. Energy schemes for the motion of a "nucleus" (a) and for the motion of an electron (b).

energies of the nucleus which correspond to a bound electron and a free electron, respectively; and $U_2(x) - U_1(x) = \epsilon_b(x)$ is the binding energy of an electron at the center. The thermal binding energy is ϵ_T, but the activation energy for the emission of an electron is $\epsilon_T + \epsilon_2$; here ϵ_2 is the potential energy of the nucleus at the point x_c, where the electron level goes out to the continuum $[\epsilon_b(x_c) = 0]$.

Above the U_2 term and parallel to it, there are the terms $U_\epsilon(x) = U_2(x) + \epsilon$, where ϵ is the energy of the emitted electron. Abakumov *et al.*[3] have shown that at the actual temperatures and not too strong electron-vibrational coupling, the thermal ionization occurs at an energy of the nucleus, E, lower than ϵ_2 by means of tunneling of the nucleus from the term $U_1(x)$ to the terms $U_\epsilon(x)$. The probability of such a transition P is determined by the overlap of vibrational wave functions and depends exponentially on the energy of the emitted electron[3] $P \sim \exp(-2\tau\epsilon/\hbar)$, where τ is the tunneling time of the nucleus in a $U_2(x)$ potential from the reversal point a_2 to the point x_c at which the terms are encountered:

$$\tau = \sqrt{\frac{M}{2}} \int_{a_2}^{x_c} [U_2(x) - E]^{-1/2} dx. \tag{1}$$

Here M is the mass of the nucleus, and E is its energy.

In an electric field an electron can undergo a transition to the continuum at $\epsilon < 0$ (Fig. 1b). The overlap of the nuclear wave functions in this case increases with increasing $|\epsilon|$. In a field, however, the overlap of electron wave functions (which is proportional to the transition probability) contains an exponential function which describes the tunneling of an electron through a triangular barrier and which decreases with increasing $|\epsilon|$. As a result, we have

$$P \sim \exp\left\{ (2\tau|\epsilon|/\hbar) - \frac{4}{3}\sqrt{2m}\,|\epsilon|^{3/2}/\hbar F \right\},$$

where F is a force which acts on the electron in an external electric field. The most probable energy of the emitted electron is determined by the maximum argument of the exponential function $|\epsilon| = F^2\tau^2/2m$, and the dependence of the probability of thermal ionization on the electric field becomes

$$e \sim \exp(F^2\tau^3/3m\hbar). \qquad (2)$$

Assuming that $U_2(x) = M\omega_2^2x^2/2$ and $E \ll \epsilon/2$, we find $\tau = [\ln 4\epsilon_2/E]/2\omega_2$ from Eq. (1). As the energy E we can insert into this expression E_0—the saddle-point energy which is determined by the competition between the probability of thermal activation of the vibrations and the probability of tunneling of the nucleus. According to Abakumov *et al.*,[3] at $E_0 \ll \epsilon_T$ we have

$$4\epsilon_2/E_0 = C\exp(\hbar\omega_2/kT),$$

where $C = [(1+\nu)/(1-\nu)]^{1/\nu}$, and $\nu = \sqrt{1-\beta}$, where β is the coupling constant which is introduced in accordance with the relation $\epsilon_b(x) = \beta M\omega_2^2(x-x_c)^2/2$. For τ we thus find

$$\tau = \frac{1}{2\omega_2}\ln C + \frac{\hbar}{2kT}. \qquad (3)$$

Equations (2) and (3) are amenable to a direct comparison with the experimental data: Figure 2 shows Tasch and Sah's[2] data on thermal emission of an electron from the acceptor level of Au in silicon into the conduction band. We see that the F dependence is in agreement with Eq. (2). The value of τ can be determined at different temperatures from Fig. 2 with the help of Eq. (2) (it is generally assumed that $m = 0.33m_0$). It can be seen from Fig. 3 that the temperature dependence of τ is well

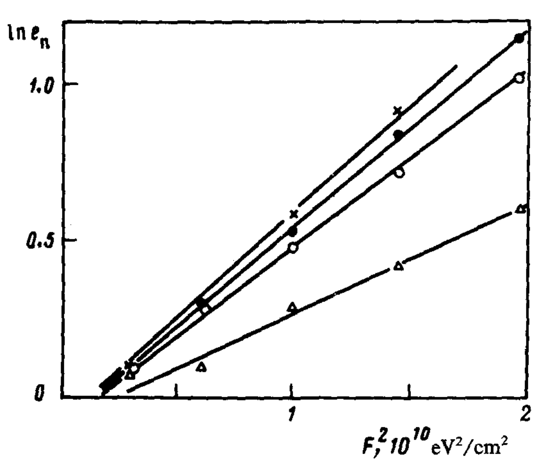

FIG. 2. The logarithm of the probability of thermal ionization of electrons from the acceptor level of Au in silicon[2] versus the square of the electric field at different temperatures. ×—197 K; ●—205 K; ○—217 K; △—283 K.

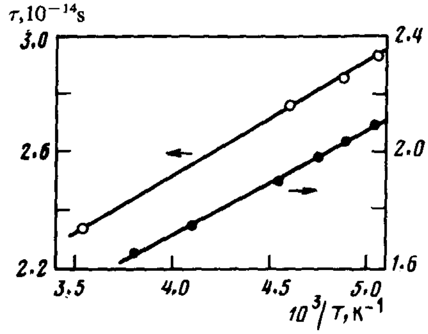

FIG. 3. The tunneling time of a "nucleus," τ, versus the reciprocal of the temperature during the emission of electrons (○) and holes (●) from the acceptor level of Au in silicon.

described by an equation which is consistent with (3):

$$\tau = \frac{\hbar}{2k}\left(A + B\,\frac{1}{T}\right), \qquad (4)$$

where $A^{-1} \cong 4.1 \times 10^2$ K, and $B \cong 1$ [according to (3) we find $B = 1$]. Also shown in Fig. 3 is a plot of τ versus T^{-1} for thermal emission of the hole from the same center in silicon to the valence band (as m we use the mass of the light hole, $m = 0.16m_0$). These data are also described by Eq. (4) with the values $A^{-1} \cong 1.3 \times 10^3$ K and $B \cong 0.9$. Analogously, B was estimated to be ~ 0.7 for the emission of holes from zinc in silicon.[4] The comparison with experiment (in particular, the fact that B is approximately equal to unity) is convincing evidence that this thermal-ionization mechanism is correct and that the reasons given for the dependence of thermal ionization on the electric field are also correct. It should be noted that the Frenkel-Pool effect may be seen in weaker fields. In the case of the attractive Coulomb centers, this effect should occur at $\sqrt{2m}\,|\epsilon|^{3/2}/F\hbar < 1$. At higher values of $|\epsilon|$ the Frenkel-Pool effect is unimportant, since the direction cone within which the electron can escape from the center without tunneling is too narrow to allow its motion to be described classically, even if the $|\epsilon|$ level is higher than the potential hump in the direction of F.[5]

We have assumed that $|\epsilon|$ is small in comparison with the typical ϵ_T and E_0 energies. We see that in fields $F \gtrsim \sqrt{2m\epsilon_T}\,\omega_2$ this condition is not satisfied. As a result, the field dependence of the probability for thermal ionization is weakened. This circumstance can conceivably account for the data on thermal ionization[6] of GaAs. In fields of even stronger intensity, a pure activation transition between the terms (without tunneling of the nucleus), which was considered by Köster *et al.*,[7] is possible.

[1]J. Frenkel, Phys. Rev. **54**, 647 (1968).
[2]A. F. Tasch and C. T. Sah, Phys. Rev. **1**, 800 (1970).
[3]V. N. Abakumov, I. A. Merkulov, V. I. Perel', and I. N. Yassievich, Zh. Eksp. Teor. Fiz. **89**, 1472 (1985) [Sov. Phys. JETP **62**, No. 4 (1985)].
[4]J. M. Herman and C. T. Sah, Phys. Stat. Sol. (a) **14**, 405 (1972).
[5]A. G. Aronov and A. S. Ioselevich, Zh. Eksp. Teor. Fiz. **74**, 1043 (1978) [Sov. Phys. JETP **47**, 548 (1978)].
[6]S. Makram-Ebeid and M. Lannoo, Phys. Rev. B **25**, 6406 (1982).
[7]H. Köster, I. N. Iassievich, and K. Hübner, Phys. Stat. Sol. (b) **115**, 409 (1983).

Translated by S. J. Amoretty