The inverson—a new type of defecton

B. L. Oksengendler

Institute of Nuclear Physics, Uzbek Academy of Sciences
(Submitted April 21, 1976)
Pis'ma Zh. Eksp. Teor. Fiz. **24**, No. 1, 12–15 (5 July 1976)

A new mechanism of defect delocalization is proposed, based on inversion of the terms and realizable with electronic transitions.

PACS numbers: 71.50.+t

Andreev and Lifshitz[1] have introduced new quasiparticles—defectons—whose quantum properties, which have been investigated from various points of view (see the reviews[2,3]), were attributed to the small mass of the atoms (H, He), which leads to a large amplitude of the zero-point oscillations.

We present below a new mechanism for the delocalization of atomic particles (which transforms a defect into a defecton under definite conditions), based on the special form of the dependence of the potential relief of the defect in the crystal on the state of an electron localized on the defect. Continuous motion of the defect is made possible by alternating transitions of the electron from the ground state to the excited state and back near definite points corresponding to term intersections.

I. We consider a nonmetal having alternating nonequilibrium interstices of two types, (H) and (T), with an interstitial defect on which the electron is

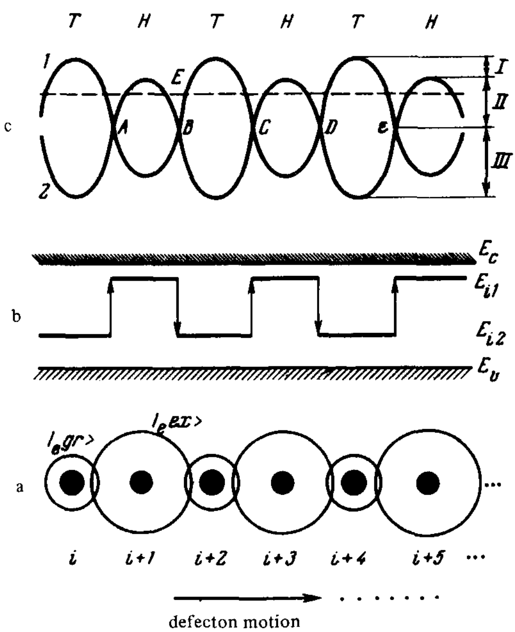

FIG. Inverson scheme: a—pattern of periodic excitation of localized electrons (black circles—"core" of defect), b—variation of the state of the localized electron in the band scheme, c—potential relief of defect in crystal (1—for excited electron and 2—for unexcited electron).

localized. Assume that this electron can be in two states: ground ($|_e gr\rangle$) and excited ($|_e ex\rangle$) (Figs. a and b), corresponding to two different potential terms that are furthermore mutually inverse (the minimum of one corresponds to the maximum of the other and vice versa) (Fig. c).[4,5] We consider the low-temperature limit $T \to 0$. Let the defect be located in the interstice numbered $i+1$ with an electron excited by an external agent in the state ($|_e ex\rangle\, |_e ex\rangle$). The potential relief of the defect is here the term 1. Moving to the right (Fig. c) in a state with total energy E, the defect can be reflected from the barrier and remain in the well $i+1$, dropping to its bottom during the course of vibrational relaxation. However, owing to the presence of the inverse term 2, when the term intersection region is reached (the point B) there is a probability (W) of the nonadiabatic electron transition $|_e ex\rangle \to |_e gr\rangle$, as a result of which the defect goes over to term 2, and the region of the interstice numbered $i+2$ becomes accessible to it. If the inverse transition $|_e gr\rangle \to |_e ex\rangle$ takes place at the point C in the course of the subsequent motion, together with the corresponding transition to the term 2, then the defect will again go over to the hitherto inaccessible region of the interstice numbered $i+3$. A continuous series of such nonadiabatic transitions leads to quasifree motion of this complex defect (atom with an electron that becomes relocalized on it) through the crystal. The corresponding quasiparticle (see below) can be logically called an "inverson." The foregoing reasoning is valid for the energy region II (Fig. c); for region I, an additional possibility of free motion is realized if there are no transitions at all (in the region above the barrier). A defecton state is impossible in energy region III.

II. Taking into account the different "inverson" decay channels, we can write down the conditions for its existence. Let $\tau_{sd} = \tau_0/W$ be the settled lifetime of the defect (τ_0 is the period of the oscillations of the atom). Then the inverson is a good quasiparticle if τ_{sd} is small in comparison with the characteristic times of defect decay via ionization or recombination, and also with the times of the relaxation of the vibrational energy of the inverson and of the direction of its quasimomentum. At low temperatures and in the absence of superdense ionization, taking the Prigogine–Bak principle into account,[6] we obtain a limit on the temperature of the inverson state: $T \ll \frac{1}{8}\Theta W^{1/9}$, where Θ is the Debye temperature.

III. In the tight-binding approximation we easily obtain from the equations for the transition amplitudes

$$|2n\rangle \equiv |H\rangle \to |T\rangle, \qquad |2n+1\rangle \equiv T\rangle \to |H\rangle:$$

$$i\hbar \dot{C}_{2n} = E_0 C_{2n} - A(C_{2n-1} + C_{2n+1}); \quad i\hbar \dot{C}_{2n+1} = E_0 C_{2n+1} - A(C_{2n} + C_{2n+2})$$

the dispersion law $E(q) = E_0 \mp 2|A|\cos qa$, where $A \approx \langle_e ex|\langle\chi_{ex}|\hat{V}|\chi_{gr}\rangle|_e gr\rangle$, with $\hat{V}$ the nonadiabaticity operator and $|\chi_{ex}\rangle$, $|\chi_{gr}\rangle$ the vectors of the (vibrational) states of the defect for the excited and ground states of the localized electron, respectively. Assuming a band width $\Delta\epsilon = 4|A| \approx \hbar/\tau_{sd}$, we obtain the estimate $M^* = \hbar\tau_0/2W\alpha^2 \approx 5\times 10^{-25}/W$ g for the effective mass. It is clear that the effective mass depends essentially on the number of the vibrational state: $M^* \sim [\langle\chi_{gr}|\chi_{ex}\rangle]^{-1}$.

IV. The diffusion properties of the inverson are analogous in many respects to the properties of the Andreev-Lifshitz light defects.[1-3,7] There are, however, some differences. If the split vibrational levels coincide, coherent diffusion predominates in the inverse terms. As applied to the inverson we obtain for the individual band $D_c \approx \overline{v^2} t_{tr} \approx (D_0/8)(\Theta/8T)^9$. For nonoverlapping levels, an important contribution is made by incoherent diffusion and by the mechanism of spontaneous emission of phonons,[8] which yield for the inverson $D_h \approx D_0(16/\omega_D \tau_0)(T/\Theta)^7$ and $D_{sp} \lesssim D_0(\gamma^2/\omega_D^4 M^2 \pi^4)$. Here $D_0 = W^2 s^2 \tau_0$ throughout (s is the speed of sound), M is the mass of the diffusant, and γ is the force constant of the terms. It is important to note that in the general case of noncoinciding levels, even in the absence of inverson scattering by the defects, the spontaneous-emission mechanism will predominate at $T < \Theta[\tau_0 \gamma^2/16\omega_D^3 M^2 \pi^4]^{1/7}$.

Notes. 1. The foregoing reasonings can be easily generalized also to the case of vacancies, dislocation kinks, split- and bond-configurations, etc. on which electronic excitations are localized and cause inversion of the terms.

2. It is possible that what was observed long ago in low-temperature ($1-20\,°K \ll \Theta$) radiation experiments on semiconductors (the problem of "long-range" migration)[9] were in fact inversons. Favoring this assumption is the agreement between the defecton model of "crowding out" of impurities by their own interstices[10] with experiment,[9] which yields the expression for the losses of the moving interstice $(-dE/dx) \ll 0.7$ eV/Å, a value much lower than the ordinary losses due to elastic collisions (25 eV/Å).

In conclusion, I am grateful to A. F. Andreev for interest in the work, for an interesting discussion, and for valuable advice.

[1]A. F. Andreev and I. M. Lifshitz, Zh. Eksp. Teor. Fiz. **56**, 2057 (1969) [Sov. Phys. JETP **29**, 1107 (1969)].
[2]A. F. Andreev, Usp. Fiz. Nauk **118**, 251 (1976) [Sov. Phys. Usp. **19**, 137 (1976)].
[3]R. A. Guyer, R. C. Richardson, and L. I. Zane, Rev. Mod. Phys. **43**, 532 (1971).
[4]B. L. Oksengendler, in: Prikladnaya yadernayafizika, Materialy aprel'skoĭ konf. molodykh uchenykh UzSSR (Applied Nuclear Physics, Proc. April Conf. of Young Scientists of UzSSR) 1971, Tashkent, "Fan," p. 221, 1973; in: Metod radiatsionnykh vozdeistviĭ v issledovanii struktury i svoĭstv tverdykh tel (Method of Radiation Effects in the Investigation of the Structure and Properties of Solids), Tashkent, "Fan," p. 16, 1971.
[5]J. Bourgoin and J. Corbett, Phys. Lett. **A38**, 135 (1972).
[6]J. Prigogine and T. Bak, J. Chem. Phys. **31**, 1368 (1972).
[7]Yu. Kagan and M. I. Klinger, J. Phys. C **7**, 2791 (1974).
[8]A. F. Andreev and A. E. Meĭerovich, Zh. Eksp. Teor. Fiz. **67**, 1559 (1974) [Sov. Phys. JETP **40**, 776 (1975)].
[9]G. Watkins, Rad. Damage Semicond, Dunod, Paris **97**, 1965; Lattice Defects in Semicond., Ins. Phys. Conf. Ser. **23**, London, Bristol, 1, 1975.
[10]D. R. Musin, B. L. Oksengendler, and M. S. Yunusov, Izv. Akad. Nauk Uzb. SSR Ser. Fiz.-Mat. Nauk, No. 4, 67 (1975).