# New explanation of recombination-stimulated phenomena in semiconductors

M. K. Sheĭnkman
*Institute of Semiconductors, Academy of Sciences of the Ukrainian SSR*

(Submitted 21 July 1983)
Pis'ma Zh. Eksp. Teor. Fiz. **38**, No. 6, pp. 278–280 (25 September 1983)

It is shown that recombination-stimulated diffusion, breakdown of clusters, and other processes in semiconductors, which were previously associated with energy transfer by nonradiative recombination to a center, can be explained by the excitation of an electron (or hole) in the center into an antibinding orbital. Experiments on identification of the proposed mechanism are examined.

PACS numbers: 71.35. + z

A new class of nonequilibrium processes occurring in semiconductors was discovered at the beginning of the 1960s: creation or annihilation of centers as a result of generation (by light or by injection) of electrons and holes with thermal energy.[1,2] Because the energy liberated due to recombination in semiconductors (1–3.5 eV) is small, these processes do not occur in an ideal lattice, as, for example, in alkali-halike crystals,[3] but are a result of photochemical reactions between existing defects and impurities: dissociation of donor-acceptor pairs, clusters, donor associates, migration of donors from sinks in the bulk of the crystal, and association of fine donors with the formation of a deep center.[4,5] They are caused by recharging of centers participating in reactions, which changes the Coulomb interaction or molecular bond betwen the components of a complex center.[6,4]

In 1974, Lang and Kimerling[7] discovered the phenomenon of recombination-stimulated diffusion (RSD): under the conditions of recombination, some defects are annealed at an activation energy ($E_{\text{RSD}}$) that is much lower than the equilibrium ($E_T$) energy. The difference

$$E_T - E_{\text{RSD}} = E_P \tag{1}$$

turned out to be close to the depth of the electron level of the center being annealed relative to the most distant band $E_P$ (Fig. 1). This effect was later observed in a number of centers in GaAs, GaP, and SiC[8,9] which permitted refining condition (1):

$$E_{\text{RSD}} = E_T - E_P + \Delta\ , \tag{1a}$$

where the value of $\Delta$ reached 0.1 eV.[8] Other characteristic features of RSD[8,9] are: a) presence of athermal diffusion in a number of centers $E_{\text{RSD}} = 0$; b) linear dependence of the rate $R$ of RSD on the concentration of the minority carriers $n_0$; c) saturation of the dependence of the rate of RSD on the recombination rate $r$.

The obvious explanation of the RSD effect, based on Eq. (1) and given in Ref. 7 and later adopted by other investigators,[8,9] is based on the fact that the quantity $E_p$ is the energy liberated with nonradiative multiphonon capture of a carrier by a center.

  

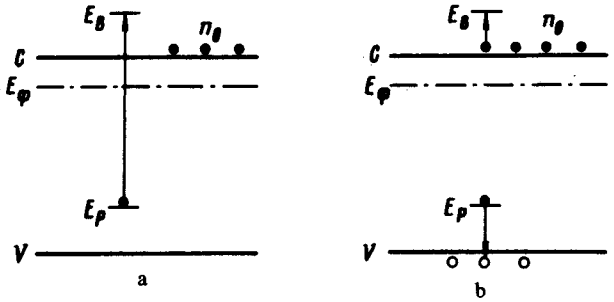


FIG. 1. Excitation of an electron out of the ground state ($E_P$) into the excited state ($E_B$) of the center, corresponding to an antibinding orbital in the following cases: a) equilibrium; b) nonequilibrium with hole injection.

This energy is completely [Eq. (1)] or partially [Eq. (1a)] transferred to the center and leads to an effective decrease in the diffusion barrier $E_T$. We note that the well-known difficulty of this explanation[8] is that the excess energy should not be dissipated in the lattice within the time of the diffusion jump.

The purpose of this paper is to show that there exists a fundamentally different, *alternative* explanation of RSD and all its characteristics that is not based on the multiphonon process. It is based on two assumptions.

1. RSD (or some other elementary process, such as decay of a DA pair, etc.) can occur at centers with a specific excited level situated in the conduction band [for example, for a deep acceptor (Fig. 1)], valence band, or forbidden band. The diffusion jump occurs with excitation of a center, when the electron makes the transition from the level $E_P$ to the level $E_B$ (Fig. 1). The level $E_B$ corresponds, for example, to an antibinding orbital. The possibility of migration of the defect accompanying excitation of a carrier into an antibinding state has been pointed out by various authors.[10–12] A calculation of the probability of such a process (dissociative attachment of an electron to a molecule), demonstrating the high probability of its occurrence, was performed in Ref. 12. In general, it turns out that with the excitation of a center, a defect in equilibrium in the lattice at the minimum of the potential energy is located at a saddle point and undergoes a diffusion jump. This the proposed mechanism is similar to Bourgoin's mechanism,[13] but for the excited rather than the recharged center.

2. The second important assumption is that equilibrium thermal diffusion of these defects occurs not according to the usual mechanism of thermal crossing of the barrier by the unperturbed center but rather by an easier route (with lower activation energy): due to thermal excitation of an electron at the center to the level $E_B$, i.e., according to the mechanisms described in Sec. 1. This gives an activation energy of equilibrium diffusion (if the Fermi level is located between the levels $E_P$ and $E_B$) (Fig. 1a)

$$E_T = E_P + E_B . \tag{2}$$

Under nonequilibrium conditions with injection of holes, the holes are captured in the level $E_P$. To excite the center, it is now sufficient that the equilibrium electron be thermally excited to the level $E_B$. Therefore, the activation energy of this process (and of the RSD process) will be (Fig. 1b)

$$E_{\mathrm{RSD}} = E_B + E_F = E_T - E_P + E_F, \tag{3}$$

where $E_F$ is the distance between the equilibrium Fermi level and the bottom of the $c$-band.

We have thus obtained the Kimerling-Lang condition (1), if $E_F \simeq 0$, and the more general condition (1a), where $\Delta = E_F$. The rate of RSD is given by

$$R \propto rw\exp\left(-\frac{E_T - E_P + E_F}{kT}\right) \propto rwn_0\exp\left(-\frac{E_T - E_P}{kT}\right), \tag{4}$$

where $n_0$ is the concentration of equilibrium electrons, and $W$ is the pre-exponential factor in the probability of a diffusion jump. It is easy to see that this process contains all the features of RSD: $R \propto n_0$; $R$ saturates with increasing $r$, accompanying saturation of centers by holes; an athermal process occurs if the level $E_B$ lies below $E_F$ in the forbidden band or in the $c$-band; capture of holes immediately leads to excitation of the center.

Important consequences of the mechanism of RSD examined above, which permit its direct experimental verification, are: 1) dependence of the activation energy $E_{\mathrm{RSD}}$ on $E_F$, in accordance with (3) and (4); 2) possibility of observing the athermal RSD process by direct optical (selective) excitation of the center: transfer of an electron from the level $E_P$ to the level $E_B$ by a quantum $h\nu = E_P + E_B$ (Fig. 1a) (this can also be done by exciting an electron to another higher-lying level with subsequent transition of the electron to the $E_B$ level); 3) possibility of observing RSD both for nonradiative and radiative recombination centers (in contrast to multiphoton mechanisms[7,8]), since capture of an electron from the bottom of the $c$-band into the $E_P$ level may be a radiative process; this situation has been observed in SiC (Ref. 9); 4) the dependence of the activation energy of equilibrium diffusion $E_T$ on $E_F$, when $E_F$ drops below the level $E_P$: $E_T = E_F + E_B$, which corresponds to recharging of the center. The dependence of $E_T$ on the charge on the center is well known for a number of centers.[8,9]

In conclusion, it is important to note that the process of athermal (or thermal, but with low activation energy) reorientation of $F_A$ centers in a KCl lattice (Cl vacancy + Na or Li atom in the neighboring cationic site) with direct optical excitation of the electron in the center into the $2s$ state, observed in 1968 by F. Luty,[14] is a good example of the recombination-stimulated process which was examined above and which was observed in a dielectric crystal. As follows from this paper, analogous processes in semiconductors should have characteristic indications of the multiphonon mechanism of RSD,[7,8] so that special study is required in all cases to discriminate them.

[1]N. E. Korsunskaya, I. V. Markevich, and M. K. Sheĭnkman, Phys. Status Solidi **13**, 25 (1966).
[2]N. E. Korsunskaya, I. V. Markevich, and M. K. Sheĭnkman, Fiz. Tverd. Tela **10**, 522 (1968) [Sov. Phys. Solid State **10**, 409 (1968)].
[3]Ch. B. Lushchik, I. K. Vitol, and M. A. Élango, Usp. Fiz. Nauk **122**, 223 (1977) [Sov. Phys. Usp. **20**, 459 (1977)].
[4]M. K. Sheinkman, N. E. Korsunskaya, I. V. Markevich, and T. V. Torchinskaya, J. Phys. Chem. Solids

**43**, 475 (1982).
[5]M. K. Sheĭnkman, N. E. Korsunskaya, I. V. Markevich, and T. V. Torchinskaya, Fiz. Tekh. Poluprovodn. **14**, 438 (1980) [Sov. Phys. Semiconductors **14**, 259 (1980)].
[6]M. K. Sheĭnkman, Pis'ma Zh. Eksp. Teor. Fiz. **15**, 673 (1972) [JETP Lett. **15**, 476 (1972)].
[7]D. V. Lang and L. C. Kimerling, Phys. Rev. Lett. **33**, 489 (1974).
[8]L. C. Kimerling, Solid State Electron. **21**, 1391 (1978).
[9]P. J. Dean and W. Y. Choyke, Adv. Phys. **26**, 1 (1977).
[10]A. E. Kiv and F. T. Umarov, Fiz. Tekh. Poluprovodn. **4**, 571 (1970) [Sov. Phys. Semiconductors **4**, 474 (1970)].
[11]V. A. Telezhkin, K. B. Tolpygo, and V. M. Shatalov, Proc. Inter. Conf. on Radiation Physics of Semiconductors and Related Materials, Tbilisi, 1979, p. 452.
[12]P. G. Eliseev, I. A. Zavestovskaya, and I. A. Poluéktov, Kvant. Elektron. **5**, 203 (1978) [Sov. J. Quantum Electron. (Moscow) **5**, 124 (1978)].
[13]J. C. Bourgoin and J. W. Corbett, Phys. Lett. A **38**, 135 (1972).
[14]F. Luty, Physics of Colour Centers, Academic Press, N. Y., 1968, p. 184.

Translated by M. E. Alferieff
Edited by S. J. Amorietty