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# Photo-stimulated Rebuilding of Structure in Semiconductors

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**Abstract**

A strong electron-phonon interaction observed in semiconductors allows to realize a special kind of atomic rebuilding under photo-irradiation of the medium. We consider three types of defective structures: one atomic, two-atomic ("dump-bell") and multi-atomic (kinks) defects. It is shown that an inversion effect of the defect potential term may be realized if there are non-equivalent neighboring positions of one-atomic and two-atomic defects. In this case the photo-excitation of electronic subsystems of these defects leads to an inversion of potential terms and a consecutive athermal rebuilding of the defective structures. The Yahn-Teller effect and psevdo-effect play a special role here. It is shown for kink-structures that the photo-excitation of the electronic subsystems results in the alteration of kink nonius and the successive exponentially strong decrease of an activation barrier. Especially effects of athermal atomic rebuilding of U-negative defects are considerable.

## Introduction

The possibility of stimulating atomic processes with electronic excitations is a new aspect of defect process physics. After the excitation of electronic subsystem the relaxation of this energy to the atomic degrees of freedom can lead to the atomic rebuilding with certain probability. Electron-stimulated atomic rebuildings (ESAR) [1,2] based on a strong electron-phonon interaction are well known in semiconductors of covalent and ionic characters. Types of such electronic-stimulated atomic rebuildings are rather wide and they can be subdivided into the small-scale and large-scale ones according to the quantity of defects involved into the atomic processes. In this work three models of ESAR based on different defects are considered in such systems.

**Body**

## 1. Photo-stimulated diffusion of one-atomic defect

Let us consider one-valent positively charged impurity atom (or host interstial atom) introducing a deep local level into the forbidden band of electronic spectra. At photo-irradiation free electron and hole are produced. This electron could be trapped on the deep local level and deform the crystal around it. The impurity atom is suggested to interact with neighbor host atoms with the following potential

$$U(r) = U_{rep}(r) + U_{attr}(r), \tag{1.1}$$

where $U_{rep}(r)$ is the repulsive energy between the ion and the neighbor host atoms, $U_{attr}(r)$ is the attractive energy between them.

The total energy of the "crystal + impurity" system for two sites of symmetry with respect to the neighbor host atoms is defined by the formulas

$$\begin{aligned} U^{(1)}(r) &= U^{(1)}_{rep}(r) + U^{(1)}_{attr}(r) \\ U^{(2)}(r) &= U^{(2)}_{rep}(r) + U^{(2)}_{attr}(r) \end{aligned} \tag{1.2}$$

The activation energy of defect for its diffusion will then be given by [3]

$$\Delta Q_m = \left| U^{(1)}(r) - U^{(2)}(r) \right| = \left| \Delta U_{rep}(r) + \Delta U_{attr}(r) \right| \tag{1.3}$$

$U_{rep}(r)$ is estimated by means of Born-Mayer`s equation:

$$U_{rep}(r) = Ae^{\frac{r_L + r_I - r}{\rho}}, \tag{1.4}$$

where A is the scalar factor, $r_L$ is the effective radius of the host atom, $r_I$ is the ionic radius of the impurity, $r$ is the distance between them, and constant ρ determines how

rapidly the repulsion falls off with distance. $U_{attr}(r)$ is connected with the effects of media polarization by the impurity:

$$|\Delta U_{attr}(r)| = |\Delta U_{pol}(r)| \leq 1эВ \quad [3]. \tag{1.5}$$

If $|\Delta U_{rep}(r)| > |\Delta U_{attr}(r)|$, then the equilibrium state of impurity will be the site (2), and the site (1) will be the saddle point.

The electron produced by photons can be trapped by the impurity. In this case according to the theory of auto-localization [4] neighbor atoms around the electron are deformed with the deformation potential which is defined from the equation

$$\rho(r) = \frac{\sigma}{k}|\Psi(r)|^2, \tag{1.6}$$

Here ρ(r) is the relative variation of volume, σ is the constant of deformation potential, k is the elastic constant, ψ(r) is the wave function of the localizing electron. To estimate the total energy of the "crystal+electron+impurity" system we have used the following expression taking into account a role of acoustic and optical phonons in the electron-phonon interaction [5]

$$E(\mu) = L\mu^2 - A\mu^3 - B\mu \tag{1.7}$$

Here μ is the parameter of localization of the electronic wave function: $\Psi(r) = \left(\frac{\mu\sqrt{2}}{a}\right)^{3/2} \exp\left[-\pi\left(\frac{\mu r}{a}\right)^2\right]$, $L = \frac{3\pi\hbar^2}{2m^* a}$, $A = \frac{\sigma^2}{2ka^3}$, $B = \frac{Ze^2\sqrt{2}}{\varepsilon a} + \frac{e^2}{a\tilde{\varepsilon}}$.

Interaction between the electron and the acoustic vibrations leads to the deformation of crystal at total localization of the electron, μ=1. In such case the repulsive energy of the impurity with neighbor atoms can be changed. For a large ion the repulsive energy will dominate $|\Delta U_{rep}(r)| > |\Delta U_{attr}(r)|$ and its activation energy of diffusion will then be defined essentially by the difference of the repulsive energies at the two sites. Therefore we can define the activation energy for its diffusion in the case of electron autolocalization

$$\Delta\tilde{Q}_m = \Delta Q_m\left(1-\frac{U_{rep}^{(1)}d^{(1)}-U_{rep}^{(2)}d^{(2)}}{U_{rep}^{(1)}-U_{rep}^{(2)}}\xi\right) \tag{1.8}$$

Here $\xi = \frac{\sigma}{3k\rho}|\Psi(r)|^2\Big|_{\mu=1} << 1$.

Thus it is clear from (1.8) that decreasing the activation energy of the defect is real at the electron localization in semiconductor.

## 2. Photo-stimulated diffusion of dumbbell defect

Semiconductor media is considered to contain a "dumb-bell" defect (two-atomic defect). It is well-known [6], that the highest engaged molecular orbital (HEMO) and the lowest empty molecular orbital (LEMO) are of even (|g>) and odd (|u>) characters, accordingly. These states are mixed as a result of the electron-ionic interaction. If the perturbation potential is defined by the equation

$$\hat{V} = \sum_i \frac{\partial V}{\partial Q_i}Q_i + \frac{1}{2}\sum_i \frac{\partial^2 V}{\partial Q_i^2}Q_i^2, \quad \text{i= g, u,} \tag{2.1}$$

using the Brulluen-Vigner`s perturbation theory at the condition of $< u|\hat{V}|u > /(\hat{\varepsilon} - \varepsilon_2) < 1$ will give the following formula for total energy of the system

$$\hat{\varepsilon} = \varepsilon_{gr} + < g|\hat{V}|g > + \frac{|< u|\hat{V}|g >|^2}{\hat{\varepsilon} - \varepsilon_u - < u|\hat{V}|u >} \tag{2.2}$$

It leads to two terms with variable catching quantities of $Q_g$ and $Q_u$. The value of total energy for the ground term $\hat{\varepsilon}_{gr}$ allows us to estimate the radius of non-stability zone (NSZ) for a displacement of the dump-bell defect as whole

$$\frac{\partial^2 \hat{\varepsilon}_{gr}}{\partial Q_n^2} \equiv F(Q_g, Q_n) = K_2 - 2a_{12}^2 \frac{\left[\Delta - (a_{11} - a_{12})Q_g\right]^2}{\left\{\left[\Delta - (a_{11} - a_{12})Q_g\right]^2 + 4a_{12}^2 Q_n^2\right\}^{3/2}} \le 0 \qquad (2.3)$$

Here $(\hat{V}Q_j' \equiv \partial\hat{V}/\partial Q_j$ et.al.) $\Delta = \varepsilon_n - \varepsilon_{gr}$, $K_1 = < g|\hat{V}Q_j''|g >$; $K_2 = < u|\hat{V}Q_j''|u >$; $a_{11} = < g|\hat{V}Q_g|g >$; $a_{22} = < u|\hat{V}Q_g|u >$; $a_{12} = < u|\hat{V}Q_n'|g >$. ZNS in neighbor interstitial sites can be overlapped. The size of ZNS is defined from the condition

$$\left|Q_g - \frac{2a_{12}^2}{a_{22} - a_{11}}\right| \le \frac{\Delta}{a_{22} - a_{11}}, \quad |Q_n - an| \le \frac{2a_{12}^2}{3\sqrt{2}K_2}, \qquad n = 0,1,2..... \qquad (2.4)$$

where a is the distance between two interstitial sites.

Let us turn to the effects of laser-stimulation of the dumbbell defect diffusion. The defect is considered to be located in the interstitial site at low temperatures and the quantum number of valence vibrations tends towards zero: $N_v \to 0$. The valence vibration amplitude begins to increase under the influence of laser. After compressing the molecule to the size of $R^* = d_0 - Q_g^*$ the transference non-stability condition appears ($d_o$ is the equilibrium length of the defect bond). The transference to the neighbor interstitial position will be realized if the valence vibrations are excited to the following threshold energy

$$E_v = \hat{\varepsilon}_{gr}(Q_g^*) - \hat{\varepsilon}_{gr}(0) + \frac{\left(\frac{\partial \hat{\varepsilon}_{gr}}{\partial Q_g}\right)^2 \tau_+^2}{2M} \qquad (2.5)$$

Here $\tau_+$ is the minimal time of impulse accumulation [2]. The time necessary for leaving ZNS is defined by $\tilde{\tau} \approx Q_g^*/(a^2 E_0/4M\omega_o)$, where $\omega_0$ is the frequency of the valence vibrations. In this case a radiation-stimulating diffusion coefficient is defined by $D \approx a^2/\tilde{\tau}$ (it can reach a value of $10^{-6}$ sm$^2$/sec).

### 3. Photostimulated diffusion of crowdion structure

Let us consider a crowdion structure characterized by its nonius. It is well-known [7] that the barrier for collective movement of the crowdion exponentially depends upon its nonius of $W_o$

$$Q_m = Q_m^o \exp\left(-\frac{\pi W_o}{a}\right) \tag{3.1}$$

where $Q_m^o$ is the diffusion barrier of one-atomic defect. Let an electron be trapped on the crowdion. The total energy of such system in the continuous approach is defined by the sum of potential energies

$$E_t\{u(x)\} = E_f + E_v + E_e \tag{3.2}$$

Here $E_f = (fa^2/2)\int_{-\infty}^{\infty}(\partial u(x)/\partial x)^2 dx$ is the potential energy of atoms in the interacted chain, f is the elasticity coefficient, $E_v = (1/a)\int_{-\infty}^{\infty} U\{u(x)\}dx$ is the potential energy of the crowdion in a field of lining; $E_e = \int_{-\infty}^{\infty}\left[(\hbar^2/2m_e)(\partial\Psi/\partial x)^2 dx + \hat{V}_{e-e}|\Psi|^2\right]dx$ is the electron energy localized on the crowdion, u(x) is the medium displacement in the crowdion wave, ψ(x) is the electron wave function. If the option of the potential energy of lining is the Eshelbi potential [8] of $U(u) = 16u_o(u/a)^2\,(1 - (u/a))^2$, and the option of u(x) is the variation function of $u(x) = (a/2)[1 - th(\mu x/a)]$, besides $\hat{V}_{e-e} = -\sum(\partial u/\partial x)$, then we have the equations

$$\begin{aligned} E_f(\mu) &= \frac{1}{6} fa^2\mu, \\ E_v(\mu) &= \frac{4}{3}\frac{U_o}{\mu}, \\ E_e(\mu) &= -\frac{\hbar^2\mu^2}{8m_e a^2}\left[-(1+2n)+\sqrt{1+\frac{4m_e\Sigma a^2}{\hbar^2\mu}}\right]^2 \end{aligned} \tag{3.3}$$

The equilibrium value of nonius of $W = 2a/\mu$ is slightly found from the condition $\partial E_t(\mu)/\partial\mu = 0$. We have the following expression at $\Sigma = 0$ (the crowdion without electron) for the crowdion nonius

$$W \to W_0 = \frac{2a}{\mu_0} = \frac{a}{(fa^2/2U_0)^{1/2}} \tag{3.4}$$

For the case of strong bond $\theta/\mu_0 >> 1$ under the condition $1 < (\mu_0/16 - 3\xi)\mu_0 - (9\xi/\theta^{1/2})\,\mu_0^{5/2}$, where $\theta = \Sigma / (\hbar^2/4m_e a^2)$, $\mu_0 = 2fa^2/U_0$, $\xi = \Sigma/8U_0$, the electron localization on the crowdion increases its nonius.

We can estimate that and receive in final

$$\tilde{W} = W_o \left[ 1 - \frac{1 - \left( \frac{\mu_o^2}{16} - 3\xi \right) \mu_o^2 - \frac{9\xi}{\theta^{1/2}} \mu_o^{5/2}}{2 + \frac{9\xi}{2\theta^{1/2}} \mu_o^{5/2}} \right] \tag{3.5}$$

As a result of that we can determine the barrier of the collective movement of the crowdion by the following formula

$$\tilde{Q}_m = Q_m \exp\left[ -\frac{\pi W_0}{a} \frac{1 - \left( \frac{\mu_o^2}{16} - 3\xi \right) \mu_o^2 - \frac{9\xi}{\theta^{1/2}} \mu_o^{5/2}}{2 + \frac{9\xi}{2\theta^{1/2}} \mu_o^{5/2}} \right] \tag{3.6}$$

It is well known that the crowdion movement can model a number of more complicated atomic rebuildings (dislocation bend movement, inter-phase border and et. al.). Therefore the analyzed relief to such collective defect as a crowdion to migrate has its wide application.

**References**

1. Deep centers in semiconductors/Ed. by S.Pantelides, N.Y.Pl.Press, 1986, 950 pp.

2. Yunusov M.S., Oksengendler B.L. et.al., Subthreshold radiation effects in semiconductors, Tashkent:Phan, 1989, 224 p.

3. Weiser K., Phys.Rew.,1962, v.126, №4, p.1427-1436.

4. Toyazawa Y. Self-trapping and defect reactions // J.Semicond. and Insulat., 1983, vol.5, p.175-200.

5. Davidov A.S., Theory of solid states, Moscow:Nauka, 1976, 639 p.

6. Toyozawa Y., A proposed model of excitonic mechanism for defect formation in Acali Halides// J.Phys.Sol.Jap., 1978, vol.44, №3, p.482-488.

7. Idenbom V.L., Frenkel-Kontorova's model with accounting the discrete structure of lattice, Kristallografia, 1957, v.3, p.197-209.

8. Seger A., Shiller P., Dislocation bends and their influence on inner friction in crystals, in: Defect influence on solid states properties / Ed. by Mezon W., v.3, chapter 8, Moscow:Mir, 1969.