# Mechanism of Electronically Enhanced Defect Reactions in Semiconductors


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Electronic transitions sometimes induce or enhance defect reactions in semiconductors, such as impurity diffusion, structural change of a defect (creation, annihilation and multiplication), and climb and glide motions of dislocation [1]. It has been suggested that the transient vibration induced by a carrier capture enhances the probability of a following capture of the opposite carrier [2,3]. Recently Shinozuka and Karatsu have simulated the transient lattice vibration induced by successive captures and it effect on the next capture process [4]. If $N$ pairs of electrons and holes are sequentially captured by a defect, each occurred at $t_{e1} < t_{h1} < t_{e2} < t_{h2} < \ldots < t_{eN} < t_{hN}$, the time evolution of $Q_1(t)$ for $t_{hN} < t$ is given by

$$Q_1(t) = Q_1^{\mathrm{before}}(t) + \bar{Q}_1 \{ -\sum_j^N \exp[-\Delta\omega^2 (t - t_{ej})^2 / 4] \cos\omega_0 (t - t_{ej}) + \sum_j^N \exp[-\Delta\omega^2 (t - t_{hj})^2 / 4] \cos\omega_0 (t - t_{hj}) \}, \quad (1)$$

for a system whose phonon frequency $\omega_k$ distribution is given by a Gaussian with the central frequency $\omega_0$ and the width $\Delta\omega$. Here $Q_1^{\mathrm{before}}(t)$ is the time dependence if all the captures of $N$ electron-hole pairs would not have occurred at all. Thus, $Q_1(t)$ is shown to be a linear combination of damping oscillations, each starts at time $t_{ej}$ or $t_{hj}$ and lasts in the same duration $\tau \sim 2\pi/\Delta\omega$. It should be reminded that the capture time $t_{ej}$ and $t_{hj}$ do not take an arbitrary value but should be obeyed by probability.

We will discuss the effect of the transient vibration (eq. 1) to defect reactions using following assumptions:

a) The first electron capture takes place by a thermal activation $Q_1$ to $Q_e$ with the activation energy $E_e^{\mathrm{act}}$.
b) If $Q_1(t)$ crosses at $Q_e$ ($Q_h$), there is a probability $p_e$ ($p_h$) per time to capture an electron (hole) nonradiatively. $p_e$ ($p_h$) ~ $\omega_{□}/2\pi$ in the adiabatic limit.
c) The defect reaction coordinate is given by $Q_R(t) = \sum_k f_k q_k(t)$, whose frequency distribution is a Gaussian with the central frequency $\omega_R$ and the width $\Delta\omega$.
d) If $Q_R(t)$ crosses the critical point $Q_c$, the defect reaction takes place.

We have found that every capture process enhances the vibration of $Q_1(t)$. On the other hand, it is not so for $Q_R(t)$ in $\omega_0 \neq \omega_R$ case, because the timing of push and pull for $Q_R(t)$ is out of phase (Fig.1).

Let us discuss the possibility of recombination-enhanced defect reaction in connection with the transient induced lattice vibration. The condition for the coherent captures turns out to be $p_e\tau$□~ $p_h\tau$ ~□$\omega_{□}$□$\Delta\omega>1$. Then if $N$ pairs of electron and hole are captured within a short period $\sim 2\pi/\Delta\omega$, the amplitude of the interaction mode $Q_1(t)$ increases remarkably. If the central frequency $\omega_{□}$□□of the reaction coordinate $Q_R$ is not so much different from $\omega_{□}$□ of the interaction mode $Q_1$, more than the band gap energy $E_g = E_e^{\mathrm{th}} + E_h^{\mathrm{th}}$ can be transformed by a series of coherent carrier captures into the lattice vibration energy. The defect reaction rate is given by $(\omega_{□}/2\pi)\exp(-E_i^{\mathrm{act}}/k_BT)$ because only the first capture ($i$=e, h) is to be activated. On the other hand, if $\omega_R$□□is much different from $\omega_{□}$□ the rate is $(\omega_{□}/2\pi)\exp(-U_0^*/k_BT)$ with $U_0$-$(E_i^{\mathrm{act}}+E_i^{\mathrm{th}})$ because the $N$ phonon-kick's are out of phase.

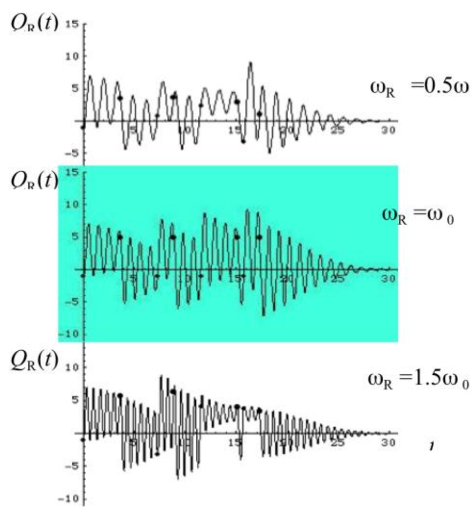


**Fig. 1** The time evolution of $Q_R(t)$. Large (small) circle indicates the capture time $t_{ei}$ ($t_{hi}$) for an electron (hole).


1. O. Ueda, "Reliability and degradation of III-V optical devices" (Artech House Publishers) 1996.
2. Y. Shinozuka, *Defects in Optoelectronic Materials*, ed. K. Wada and S. W. Pang (Gordon and Bleach Science Publisher, 2001) Chapter 8.
3. Y. Shinozuka: J. Phys. Soc. Jpn. **51** (1982) 2852 ; Jpn. J. Appl. Phys. **32** (1993) 4560.
4. Y. Shinozuka and T. Karatsu: Physica B**273-274** (1999) 999.