(We-P-21) NONRADIATIVE TRANSITIONS IN SEMICONDUCTORS — A GENERAL FORMULA FOR AN n-MODE MODEL: THE ROLE OF PROMOTING AND ACCEPTING MODES*

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A general formula is derived for multiphonon transitions assuming n different phonon modes which interact with deep centres in semiconductors. As special cases one can obtain the well-known expressions for the single mode approximation as well as a formula for the transition rate in the presence of promoting and accepting modes. The formula can be used for the calculation of the field-dependent thermal emission rate at deep centres.

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1. Introduction

Usually, the transition probability for nonradiative transitions in crystals with deep levels is calculated by assuming multiphonon processes which ensure the energy conservation for converting of the energy difference between different electronic configurations into lattice vibrational energy [1, 2, 3, 4]. Changing from extended conduction band states to the localized deep centre state, the electron stimulates the lattice to react and to find a new equilibrium position by exciting a certain number of phonons or, otherwise, the electron can be thermally excited from the deep centre to the conduction band due to a process assisted by an equivalent number of phonons. This general picture remains valid also for electric-field assisted nonradiative transitions [5] or phonon assisted tunneling [6] which results in an enhancement of the thermal emission rate. The nonradiative transition can be assumed to be made up of two processes characterized by different phonon modes which can act as promoting or accepting ones [2–4]. The promoting mode induces the transition between different electronic states and accepting modes balance the electronic energy with the vibrational energy in the relaxation process mentioned above.

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Therefore, making use of such a model one has to deal at least with two different types of modes. We will derive the formula for the transition rate in the presence of two kinds of phonons from a general expression, which has been obtained for any number of different modes taken into account in the diagonal as well as in the nondiagonal part of the electron--phonon interaction operator. The results can be used for the calculation of the nonradiative transition rate.

2. Theory

The general expression for the nonradiative thermal emission rate is [7]

$$e_n = \frac{1}{\hbar^2} \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} dE' \tilde{D}(E, E') \sum_{j,j'=1}^{n} f_j f_{j'}^{*} I_{jj'}(E, E'), \tag{1}$$

where $f_j \sim \langle c\vec{k}|V_j(\vec{x})|v\vec{k}\rangle$ is given by the nondiagonal part of the electron-phonon interaction operator. $\tilde{D}(E, E')$ is the combined density of states for the transition $E \to E'$ from the centre to the conduction band states [7]. $I_{jj'}(E, E')$ reads as follows

$$I_{jj'}(E, E') = \int_{-\infty}^{\infty} dt e^{\frac{i}{\hbar}t(E-E'-E_{\mathrm{rel}})} [D_j(t)\delta_{jj'} + Q_j(t)Q_{j'}^{*}(-t)]L(t), \tag{2}$$

with

$$D_j(t) = (N_j+1)e^{-i\omega_j t} + N_j e^{i\omega_j t} \tag{3}$$

$$Q_j(t) = \{2-[N_j(e^{i\omega_j t}-1)-(N_j+1)(e^{-i\omega_j t}-1)]\}\sqrt{S_j}, \tag{4}$$

$$L(t) = \exp\{\sum_r S_r[(N_r+1)e^{-i\omega_r t} + N_r e^{i\omega_r t} - (2N_r+1)]\}, \tag{5}$$

$$E_{\mathrm{rel}} = \sum_r S_r \hbar\omega_r.$$

N_j are the mean occupation numbers of phonon states, S_j is the Huang–Rhys factor corresponding to the j-th phonon mode with the energy $\hbar\omega_j$.

We obtain for the lattice response component $S_{\mathrm{ep}}(E, E') = \sum_{jj'} f_j f_{j'}^{*} I_{jj'}(E, E')$ without further approximations

$$S_{\mathrm{ep}}(EE') = \exp\left\{-\sum_{r=1}^{n} S_r(2N_r+1)\right\} \sum_{k_1 k_2 \ldots k_n = -\infty}^{\infty} \left|\sum_{\mu=1}^{n} f_\mu \sqrt{S_\mu}\left(1+\frac{k_\mu}{S_\mu}\right)\right|^2$$

$$\times \prod_{v=1}^{n} \left(\frac{N_v+1}{N_v}\right)^{k_v/2} I_{|k_v|}(2S_v\sqrt{N_v(N_v+1)})\delta\left(E-E'+\sum_{s=1}^{n}\hbar\omega_s k_s - E_{\mathrm{rel}}\right), \tag{6}$$

where $I_{|k_v|}(z)$ is the Bessel function.

3. Discussion

We can now immediately obtain the well-known expression in the usual single mode approximation by setting $f_1 \neq 0, S_1 \neq 0, f_v = 0, S_v = 0$ for $v > 1$. The result is

$$S_{\mathrm{ep}(1)} = \exp\{-S_1(2N_1+1)\} \sum_{k_1=-\infty}^{\infty} |f_1 \sqrt{S_1}\,(1+k_1/S_1)|^2 I_{|k_1|}(2S_1\sqrt{N_1(N_1+1)})$$

$$\times \left(\frac{N_1+1}{N_1}\right)^{k_1/2} \delta(E-E'+k_1\hbar\omega_1-E_{\mathrm{rel}}). \tag{7}$$

Assuming a promoting and an accepting modes one has to put $f_2 \neq 0, S_2 = 0$ for the promoting mode, because S_v is determined by the diagonal part of the electron-phonon interaction operator and, consequently, it vanishes for the promoting mode. On the other hand, for the accepting mode it follows from the same argumentation concerning the diagonal part of the electron-phonon interaction operator that $f_1 = 0$ and $S_1 \neq 0$. Therefore, we obtain

$$S_{\mathrm{ep(acc,prom)}} = \exp\{-S_1(2N_1+1)\} \sum_{k_1=-\infty}^{\infty} f_2^2 \left(\frac{N_1+1}{N_1}\right)^{k_1/2}$$

$$\times I_{|k_1|}(2S_1\sqrt{N_1(N_1+1)})\,[(N_2+1)\delta(E-E'+k_1\hbar\omega_1-\hbar\omega_2-E_{\mathrm{rel}})$$

$$+N_2\delta(E-E'+k_1\hbar\omega_1+\hbar\omega_2-E_{\mathrm{rel}})]. \tag{8}$$

Comparing (7) and (8) it follows that the different approximations lead to a remarkable change of the transition rate. It should be stressed that both formulas result from the same more general expression (6). Furthermore, our result is in agreement with the formula obtained recently by Perlin and Kaminskii [8].

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