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NON-RADIATIVE TRANSITION RATES: ACCEPTING AND PROMOTING PHONON MODES IN AN N-MODE MODEL

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The emission rate from deep levels due to multiphonon processes is calculated in the presence of an electric field adopting an N-mode model for the lattice vibrations. A closed analytical formula is obtained for any number of promoting and accepting modes. Experimental data on Si:Au are interpreted by means of this formula.

1. INTRODUCTION

Transitions between localized and band states induced by lattice vibrations are known to be the most important mechanism of radiationless processes in semiconductors and insulators. The quantum mechanical transitions between the initial and final electron states are caused by the non-diagonal part of the electron-phonon interaction, whereas the diagonal part makes that the transitions take place with the simultaneous excitation and deexcitation of a certain number of phonons, balancing the electronic energy change. For a given phonon mode one of these parts may dominate over the other. If this happens one distinguishes between promoting (non-diagonal part essential) and accepting modes (diagonal part essential). A theory of multiphonon transitions is needed in this case which takes more than one mode into account. Such a theory has been developed by several authors[1], restricting however to the minimum number of modes, i.e. two. In this paper we present a closed expression for the transition rate which is valid for any number of promoting and accepting modes. The expression holds also in the presence of an external electric field. It is known that the latter can cause remarkable changes of the transition rate via phonon assisted tunneling (PAT) and/or field assisted multiphonon transitions (FAMT)[2]. Whereas in PAT the role of promoting modes is played by the non-diagonal part of the electric field interaction, both accepting and promoting modes are involved in FAMT. PAT can be shown to be much less effective than FAMT for not too strong electric fields. In the present paper we concentrate ourselves on the latter process. We use our theoretical results for an analysis of experimental data on electric field dependent emission rates of Si:Au[2].

2. THEORY

We consider the emission rate e_n of an electron captured at a deep centre of binding energy E_B into the conduction band due to multiphonon and electric field induced processes. The following general expression for e_n can be derived:

$$e_n = \frac{1}{\hbar^2} \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} dE' \; D(E, E') \; \Phi(E', E) \quad . \qquad (1)$$

Here $D(E,E')$ means the electronic part of the transition probability from a localized state at energy E into a band state at E', and $\Phi(E',E)$ is the corresponding lattice part. Closed expressions are known for $\Phi(E',E)$ in the case of one promoting and one accepting mode, including the case that one and the same mode is both pro-

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moting and accepting. A closed expression can also be obtained for an arbitrary number of modes. It reads

$$\Phi(E',E) = \exp\Big(-\sum_{r=1}^{n} S_r(2N_r + 1)\Big) * \sum_{k_1,k_2,..k_n=-\infty}^{+\infty} \Big| \sum_{m=1}^{n} f_m \sqrt{S_m}\,(1 + \frac{k_m}{S_m}) \Big|^2 * \prod_{l=1}^{n} \Big(\frac{N_l + 1}{N_l}\Big)^{\frac{k_l}{2}} I_{|k_l|}\big(2S_l\sqrt{N_l(N_l+1)}\big) * \delta\Big(E - E' + \sum_{s=1}^{n} \hbar\omega_s k_s - E_{rel}\Big) \quad . \qquad (2)$$

Here the following symbols are used: $\hbar\omega_i$-phonon energy of mode i, S_i Huang-Rhys factor, N_i-phonon occupation number, f_i-non-diagonal matrix element of electron-phonon interaction, $I_n(z)$-nth modified Bessel function, E_{rel}-lattice relaxation energy.

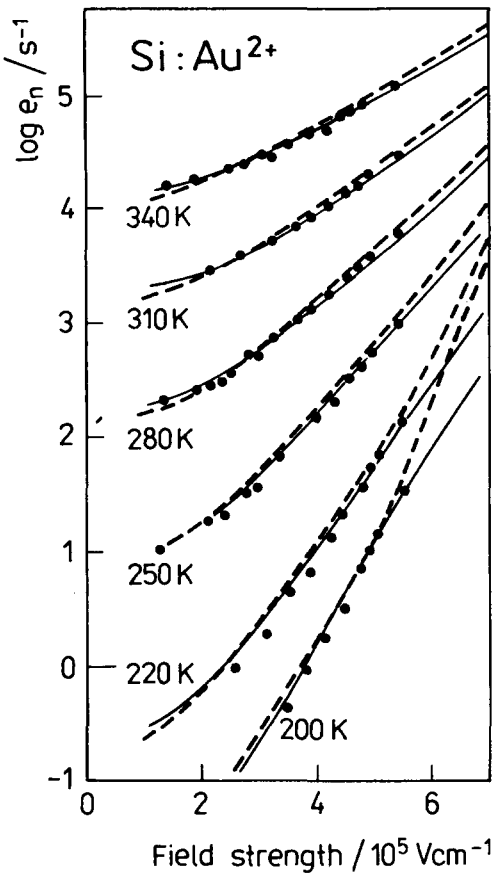

FIGURE 1
Field dependent emission rate of the Au^{2+} acceptor in Si. Experimental points from[1], theoretical curves for one-mode (dashed line) and two-mode models (full line). The following parameters are used for the one-mode model (i=0): $\hbar\omega_0$=0.068eV, S_0=2.4, E_B=(0.553eV-1.54 kT), and for the two-mode model $\hbar\omega_1$=0.070eV, $\hbar\omega_2$=0.068eV, E_B=(0.553eV -2.7 kT), S_2= 3.8

3. APPLICATIONS

We apply expression (2) to a two-mode model, i=1,2, where mode 1 is of promoting type, i.e. $f_1 \neq 0$, S_1=0, and mode 2 of accepting type, i.e. f_2=0, $S_2 \neq 0$. The resulting expression is used for the reinterpretation of experimental data on the Au^{2+}-centre in Si which so far[2] have been analysed in a one-mode model. As can be seen from Figure 1 good agreement between theory and experiment can be stated in the whole range of temperatures and field strengths. In particular, the failure of the one-mode model at low temperatures and high fields is removed.

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