(Mo-P-22) FIELD-DEPENDENT EMISSION RATE AT DEEP CENTRES IN GaAs BY USING A TWO PHONON MODE MODEL*

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The electric field dependent thermal emission rate at deep centres in semiconductors is calculated by assuming multiphonon transitions assisted by tunneling. The theory has been used to obtain the characteristic parameters, the Huang–Rhys factor and the effective phonon energy, for the EL2 centre in gallium arsenide. From the results it can be concluded that one has to add a second phonon mode in order to remove the discrepancies which result from the usual Einstein approximation.

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1. Introduction

The electric field dependent thermal emission rate at deep centres in semiconductors has been studied by assuming the phonon assisted tunneling [1] and multiphonon transitions assisted by tunneling [2, 3]. The theory has been used to obtain the characteristic centre parameters, the Huang–Rhys factor S and the effective phonon energy $\hbar\omega_p$, from the DLTS (deep level transient spectroscopy) data reported for the gold related acceptor and the A-centre in Si [4] and the EL2 centre in GaAs [1]. For the gold related acceptor in Si it has been found that $S = 2.4$ and $\hbar\omega_p = 0.068$ eV [2, 3]. These results are in agreement with the parameters obtained by Morante et al. [5] from capture measurements.

In the case of the EL2 centre in GaAs we have performed a fitting of the experimental data from [1] using the parameters $S = 6.9$ and $\hbar\omega_p = 0.02$ eV reported in [1]. We have found an agreement only for a small temperature range (see Fig. 1).

In [2] it was proposed to assume a second phonon mode in order to remove these discrepancies. We will now demonstrate how this assumption can be supported. First, we will review the results obtained in the single mode approximation, and, secondly, we will calculate the emission rate in the two mode approximation.

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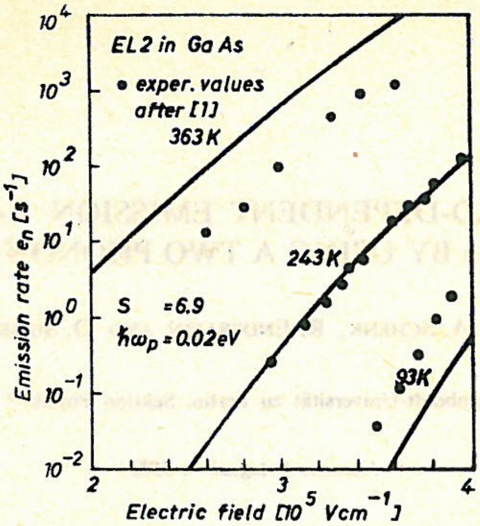

Fig. 1. Emission rate e_n for the EL2 centre in GaAs. Parameters S_1, $\hbar\omega_1$ after [1]

2. Theory

Following Lucovsky [6] and Vinogradov [7] a theory has been developed for the emission rate at deep centres in the presence of an electric field accompanied by multiphonon processes [2, 3, 8]. We obtain in the single mode approximation

$$e_n = \frac{1}{\hbar^2} \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} dE' [r_F^2 + r_p^2(E-E')] D(E, E') \phi(E'-E-S\hbar\omega_p) \tag{1}$$

where $D(E, E')$ is the combined density of states for the transition $E' \to E$ from the centre to the field modified conduction band states [2, 3]. $\phi(E'-E-S\hbar\omega_p)$ is the Fourier transform of the lineshape function known from the multiphonon theory [9]. r_F^2 and $r_p^2(E-E')$ denote the contributions to the emission rate caused by the electric field operator and the electron-phonon interaction operator, respectively. The first contribution was studied in [1] (phonon assisted tunneling).

Assuming an additional phonon mode which should interact with the centre one has to start from that general expression for the phonon contribution which is valid for any number of phonon modes. Then we obtain

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

where $f_j \sim \langle c, k | V_j(\bar{x}) | v, k \rangle$ is given by the matrix element of the electron-phonon interaction operator from the band states, because the centre wave function is built up by the valence band states (see [8]). $\tilde{D}(E, E')$ is the corresponding combined density of states for the transition from the centre to the field modified conduction band states. $I_{jj'}(E, E')$ reads as follows

$$I_{jj'}(E, E') = \int_{-\infty}^{\infty} dt e^{\frac{i}{\hbar}t(E-E'-E_{rel})} [D_j(t)\delta_{jj'} + Q_j(t)Q_j^*(-t)]L(t), \tag{3}$$

where

$$D_j(t) = (N_j+1)e^{-i\omega_j t} + N_j e^{i\omega_j t}, \tag{4}$$

$$Q_j(t) = \{2-[N_j(e^{i\omega_j t}-1)-(N_j+1)(e^{-i\omega_j t}-1)]\}\sqrt{S_j}, \tag{5}$$

$$L(t) = \exp\{\sum_r S_r[(N_r+1)e^{-i\omega_r t} + N_r e^{i\omega_r t} - (2N_r+1)]\}, \tag{6}$$

$$E_{rel} = -\sum_r S_r \hbar\omega_r. \tag{7}$$

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 $\hbar\omega_j$.

Specializing the general expressions (3)–(7) for the case of two phonon modes one has $j, j' = 1, 2$. Expanding the exponential terms appearing in $L(t)$ in rows one obtains the well-known representations in terms of the Bessel functions $I_\nu(2S_j\sqrt{N_j(N_j+1)})$. After some algebra the prefactors of the Bessel functions of different index can be combined and the final result is

$$e_n = \frac{2\pi}{\hbar^2}\int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} dE'\tilde{D}(E, E')S_{ep}(E', E) \tag{8}$$

with

$$S_{ep}(E', E) = \sum_{k_1=-\infty}^{\infty}\sum_{k_2=-\infty}^{\infty} |f_1\sqrt{S_1}(1+k_1/S_1)+f_2\sqrt{S_2}(1+k_2/S_2)|^2 \times \left(\frac{N_1+1}{N_1}\right)^{\frac{k_1}{2}}\left(\frac{N_2+1}{N_2}\right)^{\frac{k_2}{2}}$$
$$\times I_{k_1}(S2_1\sqrt{N_1(N_1+1)})I_{k_2}(2S_2\sqrt{N_2(N_2+1)})\delta(\omega-\omega'+\omega_1 k_1+\omega_2 k_2-\omega_{rel}). \tag{9}$$

The single mode approximation follows immediately from (9) for $f_2 = 0$, $S_2 = 0$.

3. *Discussion*

Comparing the expression for the emission rate obtained in the single mode approximation (1) with (8) one can expect that in the presence of a second mode the emission rate can be enhanced or reduced in different temperature ranges, if the values of S_j and $\hbar\omega_j$ differ remarkably from each other. This is due to the Bessel functions the main contributions of which are from different ranges of the energy scale, because the number of phonons accompanying the tunnel process is determined by the ratio $E/\hbar\omega_p$. Therefore, the question which has to be answered should be, if there is a second parameter set which allows one to fit the experimental data with a reasonable agreement, i.e. with the same accuracy as reported in the previous paper [1] where the values $S_1 = 6.9$ and $\hbar\omega_{p_1} = 0.02$ eV (see Fig. 1) have been used. The result is shown in Fig. 2. In fact, taking the parameters $S_2 = 2.0$ and $\hbar\omega_{p_2} = 0.04$ eV the discrepancies in the low temperature range can be removed and, furthermore, there is an agreement between the theoretical curves and the experimental data for higher temperatures up to 363 K. However, the fitting with the new parameters reveals a new disadvantage, because the field dependence is now described with less accuracy.

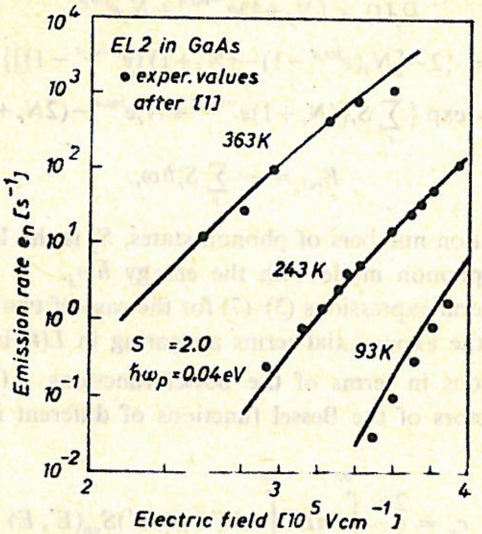

Fig. 2 Emission rate e_n for the EL2 centre in GaAs. Alternative parameter set S_2, $\hbar\omega_2$

Nevertheless, the value of the phonon energy used for the fit seems to be supported by the fact that it is close to the energy of the phonon mode $\hbar\omega_{LO} = 0.035$ eV active in GaAs. Therefore, it seems to be reasonable to study the interconnected contributions of two modes to the emission rate using formula (8). This should be necessary, because the results indicate that in the single mode approximation both the temperature dependence and the field dependence of the emission rate at the EL2 centre in GaAs can be described only with a limited accuracy.

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