THE INTERPLAY OF INITIAL AND FINAL STATE FIELD EFFECTS IN THE EMISSION RATE OF DEEP CENTRES*

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Using a quantum defect wave function and its modification in a strong field approximation, the electric field enhanced thermal emission rate at deep centres is calculated. We investigate the relative influence of the initial state field effects — lifetime broadening and Poole–Frenkel shift — in comparison with the Franz–Keldysh effect of band states. The theory is applied to the EL2 midgap level.

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1. Introduction

The field dependence of thermal emission rates (ERs) serves as a source of information about deep levels ([1, 2]). Whereas for neutral defects the initial state field effect can be neglected, a stronger modification of the wave functions is expected in the case of charged centres.

In this paper we study the influence of a field modified initial state on the ER of a charged centre. A possible explanation of the recently observed anisotropy of the ER of EL2 in GaAs [3] is the anisotropy of the Coulombic barrier giving different types of the Poole-Frenkel effect.

2. Theory

As long as the zero field ground state of the centre is primarily determined by the short range part of the defect potential, the phonon induced, field assisted ER of a donor like centre can be expressed by the formula (see [4, 5, 6])

$$e_n = \tilde{e}_n^0 e^{-S(2\bar{N}+1)} \sum_{l>0} I_l[2S\sqrt{\bar{N}(\bar{N}+1)}] \left(\frac{\bar{N}+1}{\bar{N}}\right)^{-\frac{l}{2}} \times \frac{[S-l]^2 \varrho(l, \Delta m)}{\left[\frac{\hbar\omega_0}{2\mu c_S^2} + \frac{E_B}{\hbar\omega_0}\Delta m - S + l\frac{m_c}{\mu}\right]^2}. \tag{1}$$

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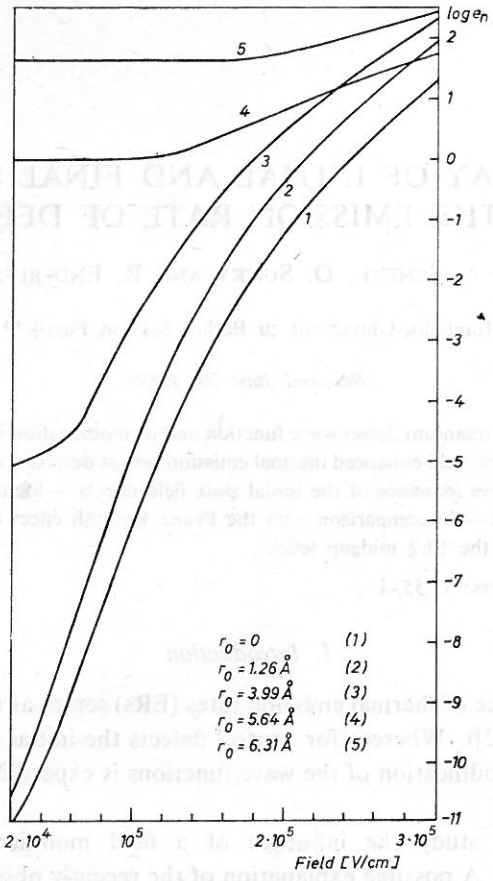

Fig. 1. Field dependence of the thermal emission rate without Poole–Frenkel shift. Curves *1–5* belong to different localization radii of the deep centre wave function. Parameters: $T = 333$ K, $S = 5$, $\hbar\omega_0 = 0.020$ eV, $Z = 1$

The notation in (1) is as follows: S — Huang-Rhys factor, $\bar{N}$ — phonon occupation number, c_S — sound velocity, E_B — binding energy, I_l — modified Bessel function. Initial and final state field effects are described by a combined density of electronic states $\varrho(l, \Delta m)$

$$\varrho(l, \Delta m) = \left(\frac{2m_c}{\hbar^2}\right)^{3/2} \sqrt{R_Z} f(l, \Delta m)$$

$$\times \left\{ \tfrac{1}{4} \int_0^\infty dt Ai\left[\frac{1}{\Delta m^{1/3}}\left(\frac{E_B^0/\Delta m + (S-l)\hbar\omega_0}{\hbar\theta_c} + t\right)\right] \exp\left[t\sqrt{\frac{E_B^0}{\hbar\theta\mu}}\,\frac{(1-\Delta m)^{2/3}}{\Delta m^{1/3}}\right] \right.$$

$$\left. + \frac{R_Z}{\pi\hbar\theta_c} \sum_{n=1}^{\infty} Ai\left[\frac{1}{\Delta m^{1/3}}\left(\frac{E_B^0/\Delta m - R_Z/n^2 + (S-l)\hbar\omega_0}{\hbar\theta_c}\right)\right] \exp\left[-\frac{R_Z}{\hbar\theta_c n^2}\right.\right.$$

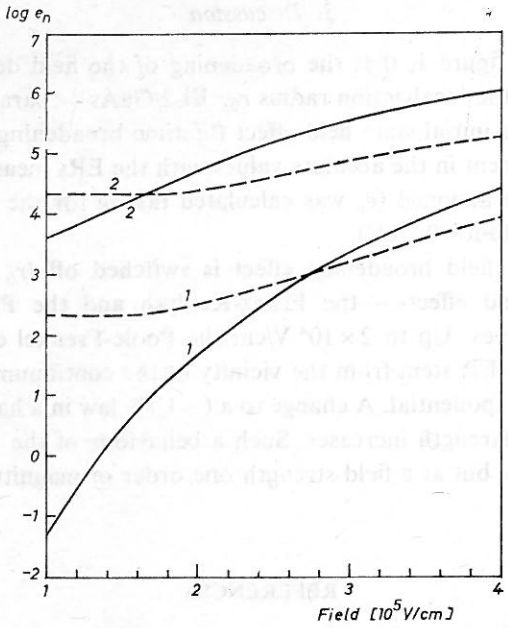

Fig. 2. Field dependence of the thermal emission rate for two different types of the Poole–Frenkel effect: (*1*) $\Delta_{PF} \sim \sqrt{F}$, $\langle\bar{1}\bar{1}\bar{1}\rangle$-direction; (*2*) $\Delta_{PF} \sim F$, $\langle 111\rangle$-direction, $q_A = 0.9e$, $q_I = 0.1e$; (———) $r_0 = 4.0$ Å; (– – – –) $r_0 = 6.3$ Å

$$\times \sqrt{\frac{E_B^0}{\hbar\theta_\mu}\,\frac{(1-\Delta m)^{2/3}}{\Delta m^{1/3}}}\Bigg]\Bigg\} \tag{2}$$

with

$$f(l, \Delta m) = \exp\left\{\tfrac{1}{3}\left(\frac{E_B^0}{\hbar\theta_\mu}\right)^{3/2}\frac{(1-\Delta m)(2+\Delta m)}{\Delta m^2} + \sqrt{\frac{E_B^0}{\hbar\theta_\mu}}\,\frac{(1-\Delta m)^{2/3}}{\Delta m^{1/3}} \times (S-l)\,\frac{\hbar\omega_0}{\hbar\theta_c}\right\}. \tag{3}$$

The field dependent initial state enters the final expression in form of the parameter $m = 1 - m_c/\mu \cdot \mu$ denotes an effective mass of the bound electron, $\hbar\theta$ the electrooptical energy, R_Z the effective Rydberg, $\hbar\theta_0$ the phonon energy, m_c the band mass and $E_B^0 = E_B - S\hbar\omega_0$. The result is based on a strong field approach ([7]) to the quantum defect initial state wave function, valid for $\hbar\theta_\mu > \hbar\omega_0$. The same approach has been applied to the Coulombic density of final states. Obviously, the initial state field effect can be switched off by $\Delta m \to 1$ (or $\mu \to \infty$), then ϱ turns to the field modified Coulombic spectrum ([5]). If the ER is plotted over the field strength, the increase of the ratio m_c/μ flats the curves drastically. This is shown in figure 1, where deep centre parameters have been used characteristic for EL2 in GaAs. The mass has been transformed into r_0 according to $E_B = \hbar^2/(2\mu r_0^2)$.

3. Discussion

It turns out from figure 1, that the broadening of the field dependent ER curves is a sensitive function of the localization radius r_0. EL2/GaAs — parameters yield the result that up to $r_0 \approx 1$ Å the initial state field effect (lifetime broadening) can be neglected. In order to achieve agreement in the absolute values with the ERs measured by Dobaczewski [3], $r_0 \approx 5$ Å has to be assumed (e_n was calculated taking for the nondiagonal electron-phonon coupling constant 10^{-2} eV).

If the initial state field broadening effect is switched off ($r_0 < 1$ Å), the interplay of two exponential field effects — the Franz-Keldysh and the Poole-Frenkel effect — determines the ER curves. Up to 2×10^4 V/cm the Poole-Frenkel effect dominates, since all contributions of the ER stem from the vicinity of the continuum edge, where the final state field effect is nonexponential. A change to a $(-1/F)$ law in a half- logarithmic picture occurs, when the field strength increases. Such a behaviour of the ER is suggested in [3] for the $\langle \bar{1}\bar{1}\bar{1} \rangle$-direction, but at a field strength one order of magnitude to large according to our theory.

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