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ELECTRIC FIELD ENHANCED THERMAL EMISSION FROM CHARGED DEEP LEVELS IN SI

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ABSTRACT

Experimental and theoretical investigations of electric field enhanced thermal emission of free carriers from charged deep levels are carried out.

1. INTRODUCTION

It is generally accepted that an accurate determination of transition rates at deep centres using methods of space charge spectroscopy (e.g. DLTS) has to take into account the influence of the inevitable electric field. Its neglection can, e.g., cause an underestimation of the zero-field activation energy. Therefore, depth-resolved measurements (e.g. DDLTS) should be carried out. The improvement of the theory upon the model of Makram-Ebeid and Lannoo /1/ has successfully been applied to neutral centres in Si by present authors /2/. For charged deep levels, however, no adequate theory is available so far. Therefore we have theoretically and experimentally reinvestigated the electric field enhanced thermal emission from charged deep centres refering to two deep Coulomb attractive centres in Si.

2. EXPERIMENT

Gold Schottky diodes were prepared from Czochralski-grown [111]-oriented, n-Si doped with P to about $6\times10^{14}cm^{-3}$. The first deep level studied here, an oxygen-related donor /3/, was produced by a short 450°C heat treatment of the starting material and labeled E1. The second deep level was generated by proton implantation at 77K (300keV, $1\times10^{10}cm^{-2}$) and labeled E3'. Since it anneals out at about 120K (Fermi-level above the E3'-level) the measurements were immediately commenced after the implantation. The electric field dependence of the ERs was

studied by a double correlation variant of capacitance transient spectroscopy to achieve the necessary depth and field resolution. Under the assumption of small deep to constant shallow doping ratios as realized in our investigation simple analytical approximations can be used to relate the emission signal to a small interval at depth x determining the field strength by $F(x) = F_0(1-x/W)$. The maximum field F_0 is reached at the metal-semiconductor interface and can be experimentally determined by the total electric potential drop and the width W of the space charge layer: $F_0=2(U_0+U_D)/W$ (U_0 is the reverse bias and U_D the built-in potential). The variation of the field strength by means of x and U_0 was applied to E1 and E3', respectively.

3. 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 can be expressed in form of a convolution integral /2/ which reads for a donor like centre

$$e_n = e_n^0 \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} dE' (E-E')^2 \frac{\varrho_t(E)\,\varrho_c(E')}{\left[\frac{\hbar^2 q_0^2}{2\mu_c} + \frac{m_c}{\mu_c} E'-E\right]^2} L_{E',E}\left(\frac{E-E'}{\hbar} - S\omega_0\right) \quad (1)$$

In (1) $\varrho_{t,c}(c)$ denote the densities of bound and final states, respectively, μ_c is the effective mass of the bound electron. Since we will restrict ourselves to the Einstein model, the line shape function of multiphonon-theory, $L_{E',E}(\omega)$ depends only on one effective phonon with frequency ω_0, q_0 is the phonon wave vector in field direction, S the Huang-Rhys-factor and I_l the modified Bessel function for integer l.

In the case of STRONG ELECTRIC FIELDS defined by $h\Theta$ R_z ($\hbar\Theta$ - electrooptical energy, R_z - effective Rydberg) an analytical approach for $\varrho_c(E')$ can be applied, which has been found by one of us in the calculation of electroabsorption spectra of excitons . On the other hand, since $\hbar\Theta \ll E_B^0$ can be assumed for deep centres, the field and Coulomb effects on the initial state should be negligible in the strong field limit. Considering attractive Coulomb potentials, both the continuous and the discrete part of the spectrum has to be taken into account in the calculation of the density of final states: $\varrho_c(E') = \varrho_c^>(E') + \varrho_c^<(E')$. Due to the assumed condition $E_B^0 \gg h\Theta \gg R_z$ only states in the exponential tail are expected to essentially contribute to the emission rate, which enables us to write $\varrho_c^>(E')$ in form of a single integral

$$\varrho_c^>(E') \sim \sqrt{R_z/\hbar\Theta_c} \int_0^{\infty} dE \left[1-\exp(-2\pi\sqrt{R_z/E})\right]^{-1} Ai^2\left(\frac{E-E'}{\hbar\Theta_c}\right)/\,E. \quad (2)$$

Relation (2) expresses the convolution of the Coulomb continuum with the spectral function $Ai^2((E-E')/\hbar\Theta_c)/E$ in a strong electric field. If R_Z tends to zero, formula (2) describes the well known Franz-Keldysh limit. In the case of discrete states an analogous relation holds if $|E'|/\hbar\Theta_c \gg 1$ is fulfilled again. In fig. 1 we have plotted the field dependent ER for three charge states and deep centre parameters characteristic for EL2 in GaAs (E_B= 0.75eV, $\hbar\omega_0$=20meV, S=5) using (1), (2).

An increasing Coulomb part of the defect potential flats the curves as a consequence of the higher density of continuum states. In the experimental range of field strength, visualized by the insert, the ERs of a neutral and a double attractive centre can deviate by a half order of magnitude. However, it is difficult to distinguish between Coulomb and multiphonon effects in a fit procedure, because variations of other parameters (e.g. binding energy by 50meV or Huang-Rhys-factor increased from 5 to 9) cause similar effects. Thus only weaker fields($\hbar\Theta \approx R_Z$) are expected to allow unambiguous decisions on the charge state.

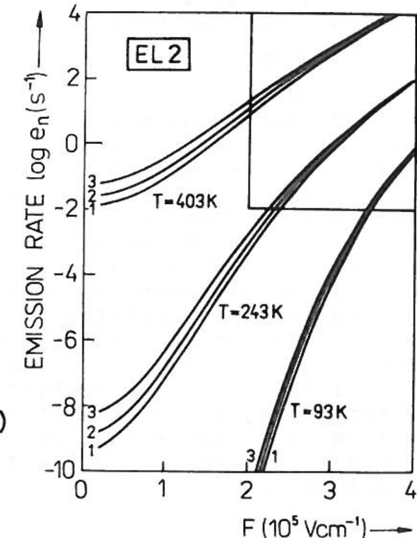

Fig.1: ER for EL2; neutral (1), 0/+(2), +/++(3)

In the WEAK FIELD case we first investigate <u>final state effects</u>. To do this, we extend the approximation (2) to the case $\hbar\Theta \lesssim R_Z$, neglecting the contributions from excited bound states. There are two arguments to accept (2) also in this case: 1. field effects on excitons were shown numerically to be well described by (2) in the region $\hbar\Theta \approx R_Z$, 2. continuum states should allow the application of (2) also in the range $\hbar\Theta < R_Z$, since for sufficiently high lying continuum states it becomes exact even for very low electric fields.

The field dependence of the ER now is fully determined by the adopted phonon model. In the case of one effective phonon mode strong variations can result depending on the ratio between $n\hbar\omega_0$ and the thermal depth E_B of the centre (n=number of phonons). Experimental data can be explained if $n\hbar\omega_0 < E_B$, but the curves are very similar for all charge states then, i.e. coincidences between electric field and phonon oscillations mask charge effects. However, taking into account phonon dispersion, the field effect almost vanishes. That happens

for all charge states, therefore, final state effects should not be responsible for the observed strong field dependence of the ER.

The investigation of initial state effects cannot be done analytically. We have estimated the influence of the short range potential on the whole potential drop in an electric field for a one-dimensional model. As it has to be expected, the contribution of the short range part is negligible for all relevant field strengths, since the maximum of the potential is located a few Bohr radii away from the origin. Thus the usual Poole-Frenkel model is applicable to deep charged centres.

4. CONCLUSIONS

In fig. 2 and 3 we have compared the experimentally observed field dependent ERs of E1 and E3' in Si, respectively, with the theoretical predictions of the Poole-Frenkel model. We use the more realistic 3-dimensional version of this model proposed by Hartke. The experimental E1-data are well described by the assumption that a transition from the + to the ++ state has been observed. This is in accordance with infrared and Hall measurements by Wruck et al. but disagrees with the DLTS-results of Kimerling et al. /3/ who have related the ER to the average junction field. The best fit for the E3'-defect can be obtained by assuming a single donor. The E3'-defect was tentatively identified as a vacancy-hydrogen complex with a nearby Si interstitial or an interstitial hydrogen atom (/4/). The following T^2-corrected (zero-field) activation energies could be extrapolated: $E_B=(132\pm5)$meV for E1 and for E3' $E=(160\pm5)$meV.

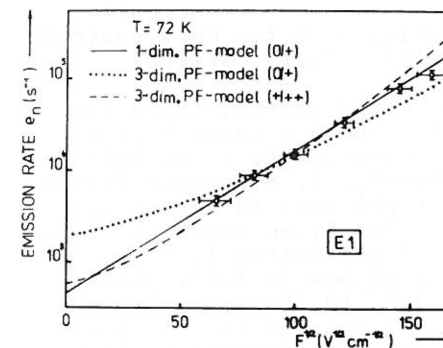

Fig.2: ER for E1

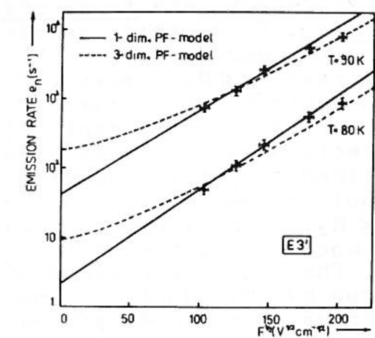

Fig.3: ER for E3'

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