(Mo-P-10) FIELD DEPENDENCE OF THE EMISSION RATE AT DEEP CENTRES IN Si AND GaAs*

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The electric field dependent thermal emission rate at deep centers in semiconductors has been studied by assuming phonon assisted tunneling and multiphonon transitions due to electron-lattice coupling assisted by tunneling. The theory has been used to obtain the characteristic parameters, the Huang-Rhys factor and the effective phonon energy, for the gold acceptor in silicon and the EL2 center in galium arsenide.

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1. Introduction

Deep centers in space charge regions of semiconductors change the characteristics of electronic devices. They are necessary for functioning of switching diodes or photodetectors but, on the other hand, they can reduce, for example the quantum efficiency of LED's due to the generation of additional recombination currents.

In the last years effective experimental techniques have been developed to detect deep centers and to determine their characteristics parameters. One of these methods is the DLTS (deep level transient spectroscopy) which allows one to study the dependence of the emission rate at deep centers on the temperature and the electric field.

The field dependence may be of interest because the field strength in the space region of junctions in electronic devices reaches values up to some 10^5 V cm^{-1}. Thus the recombination and generation of charge carriers do not only depend on the temperature but are strongly influenced by the electric field. In 1970 such a dependence of the thermal emission rate on Si : Au for a field strength in the order of $1 \cdot 10^4$ Vcm^{-1} was observed by Tasch and Sah [1]. In the last years the depleted layer spectroscopy was essentially improved and made possible the determination of the recombination parameters of deep levels with currently increased accuracy. By means of this new capacitance methods some discrepancies were established in such well-known data on gold in silicon [2]. Recently a strong

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field dependence of the thermal emission rate has been reported also on other materials, e.g. on GaAs : Cr [3], the EL2 center in GaAs [4, 5], on GaP : N [6], on Si : Au by other experimental groups [5, 7] and on the A-center in Si [7]. In contrast to the experimental results reported in [4] Kaminska et al. [8] did not observe a field dependence of the emission at high temperatures (363 K and 404 K) on the EL2 center in GaAs. The existence of the EL2 center in the crystals used was confirmed by optical measurements which have been allowed to determine the energy of the phonons interacting with the center [8].

Usually the experimentally observed enhancement of the emission rate has been interpreted by invoking the Poole–Frenkel effect [6] or by phonon-assisted tunneling mechanism (Makram–Ebeid et al. [4]). The last mechanism describes the temperature dependence using the multiphonon theory which is well-known from the theory of optical spectra and radiationless transitions [9, 10]. Therefore, by fitting DLTS-data one can obtain the values of the Huang–Rhys factor S and the characteristic (effective) phonon energy $\hbar\omega_p$. In the case of the EL2 center in GaAs Makram–Ebeid et al. have obtained the folowing parameters, $\hbar\omega_p = 20$ meV for the phonon energy and $\Delta_{FC} = S\hbar\omega_p = 140$ meV for the Franck–Condon shift. Is should be mentioned that the theoretical value of the Franck–Condon shift, and, therefore, the value of S depend on the models used by the authors in different versions of their theory (see paper [4]).

The value of the phonon energy reported by Kaminska et al. [8] for the EL2 centre is $\hbar\omega_p = 11$ meV and was obtained from the low temperature (8 K) optical absorption spectrum for the EL2 intracenter transition.

Another controversial result concerning the parameters S and $\hbar\omega_p$ has been reported by Irmscher et al. [7] who obtained from their DLTS data on Si : Au by using an earlier version of Makram–Ebeid theory [4] the parameters $S = 15$ and $\hbar\omega_p = 10$ meV, whereas the values of these parameters reported in literature are $S = 2.4$ and $\hbar\omega_p = 68$ meV [11]. Such a strong deviation is not to be expected from the theory because the value of the phonon energy remains the same for different versions of the theory (see paper [4]).

It should be stressed that Makram–Ebeid et al. [4] used a high temperature approximation which seems to underestimate the emission rate in temperature range above 250 K. In this paper we develop a theory which is valid for the whole temperature range without approximations in the high temperature range. Using this theory we are able to remove the discrepancies concerning the parameters of the gold center in silicon.

2. *Theory*

Following Lucovsky [12] and Vinogradov [13] we calculate the wave functions in the presence of an electric field. By assuming a parabolic band structure the problem can be solved exactly if we neglect the coupling between different bands. Then the Schrödinger equations for the envelope functions of the conduction band states and the impurity states read as follows

$$\left[-\frac{\hbar^2}{2m_c}\nabla_{\bar{x}}^2 - eFz - E\right]\phi_E^c(\bar{x}) = 0, \tag{1}$$

$$\left[-\frac{\hbar^2}{2m_v}\nabla_{\bar{x}}^2 - V_{\text{imp}}(\bar{x}) - E - E_g\right]\phi_E^t(\bar{x}) = 0, \tag{2}$$

where

$$V_{\text{imp}}(\bar{x}) = V_0\delta(\bar{x})\,(1+\bar{x}\cdot\nabla_{\bar{x}})$$

is the impurity potential taken after Vinogradov [13]. F is the electric field. E_g denotes the energy gap. In the field-free case Eq. (2) gives one localized eigenstate in the gap at an energy $E = -E_g+E_B$. The field broadens the corresponding δ-peak in the one electron density of states and leads to contributions over the whole range of the energy scale. Nevertheless, we can neglect the field influence on the impurity state in comparison to the field effect on band states bacause the δ-like character of the peak is preserved for field strength up to $5\cdot 10^5$ Vcm^{-1} (see [14]).

Combining the contributions from the conduction band and the impurity we obtain for the combined density of states for the transition $E' \to E$

$$D(E, E') = \frac{2}{\pi}\left(\frac{m_c}{m_v}\right)^{3/2} \mathrm{P}\,\frac{1}{\left[\frac{m_c}{m_v}E+E_B\right]^2}\sqrt{E_B}\,\mathcal{N}_c(E')\delta(E'+E_g-E_B). \tag{3}$$

P indicates the principle value. $\mathcal{N}_c(E)$ is the field-modified density of states of the conduction band.

The coupling of the electronic state to the lattice is described in the adiabatic approximation by using the static eigenstates of the electronic subsystem. The validity of different coupling schemes has been extensively discussed in literature (see, for example, [14–18] and the papers cited therein). The result was that all decoupling schemes give identical results if one restricts the calculation to contributions in the first order of the perturbation theory with respect to the linear electron-lattice coupling operator [17]. We obtain for the emission rate e_n the following expression.

$$e_n = \frac{1}{\hbar^2}\int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} dE'[r_F^2 + r_p^2(E-E')]D(E, E')\phi(E'-E-S\hbar\omega_p). \tag{4}$$

$\phi(\Omega)$ is the Fourier transform of the lineshape function known from the multiphonon theory [9, 10]. Eq. (4) describes two emission processes, the first one is induced by the electric field and is characterized by the coefficient r_F. This process was studied by Makram–Ebeid et al. [4] (phonon assisted tunneling). The second one is induced by the electron-phonon interaction (tunneling enhanced multiphonon transition) and is characterized by the coefficient r_p. In Eq. (4) both processes are described by the same function $\phi(\Omega)$. This result is valid only by assuming the Einstein approximation. The second contribution gives in the limit $F \to 0$ the rate of thermal emission e_{n0} which is automatically included in our theory.

3. Comparison with experiment

Using Eq. (4) we can calculate the field dependent emission rate for deep centers in Si and GaAs. Assuming the parameters reported in literature we obtain good agreement of the theoretical and experimental results for Si in the whole temperature range, whereas for GaAs such an agreement could be obtained only for temperatures up to 250 K. For the EL2 center we obtain good agreement for temperatures up to 250 K using the parameters $S = 3.5$ and $\hbar\omega_p = 0.02$ eV for the fit of the theoretical curves to the experimental data reported by Makram–Ebeid et al. [4]. For high temperatures we obtain only a weak field dependence of the emission rate. Therefore, the experimentally observed weak field dependence of e_n reported by Kaminska et al. [8] may be explained by our theory. Recently Dobaczewski has observed an anisotropy of the field dependence of the emission rate at the EL2 center in GaAs [19]. Therefore, it should be necessary to take into account a more complicated impurity model. On the other hand, the theoretical results are in good agreement with the experimental data reported by Irmscher et al. for Si : Au [7] if we use the parameters reported by Norante et al. [11], i.e. $E = E_c - 0.55$ eV, $S = 2.4$ and $\hbar\omega_p = 0.068$ eV, and a value $m^* = 0.42$ m for the effective conduction band mass (instead of the value $m^* = 0.24$ m which results for the (111)-direction in Si). This disagreement may be explained by the simplified band structure assumed in our model which describes only in a rough approximation the real band structure of the host material.

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