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ELECTRIC FIELD EFFECT ON MULTIPHONON TRANSITIONS AT DEEP CENTRES

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1. Introduction

It has been demonstrated both experimentally and theoretically that multiphonon transitions from deep levels into band states, under certain conditions, are extremely sensitive to an applied electric field. The effect has been clearly seen in the case of the EL2 centre in GaAs /1/ and of the Au-related neutral acceptor in Si /2,3/. In the case of GaAs a good level of theoretical understanding has already been reached by the work of Makram-Ebeid et.al. /1/ although there remain unresolved problems also in this case. In comparison to GaAs the situation for Si is more complex due to the indirect gap, the multi-valley structure and effective mass anisotropy of the conduction band. It is the purpose of this paper to develop a theory of the electric field effect on multiphonon emission which applies also to the more complex situation of Si. Further we will present experimental results on field dependent emission rates from the neutral Au-acceptor and the A-centre in Si and give an adequate theoretical interpretation for them. The authors of /1/ constructed their theory of multiphonon transitions in an electric field by extending the theory of tunneling between gap and band states to the case where multiphonon transitions can take place in addition, i.e. where tunneling processes become phonon-assisted. In this paper we start from the standard theory of multiphonon transitions and extend it to the case where an electric field is present. In this way the various field effects considered so far, like phonon assisted tunneling and Poole-Frenkel effect, are automatically taken into account, but additional effects are also regarded like tunneling enhanced multiphonon transitions, Stark effect and field induced line shape broadening of the deep level. In part 2 of the paper we present the theory. In part 3 we describe the experimental procedure. A comparison between theory and experiment is made in part 4. Some unresolved problems in the case of the EL2 centre in GaAs are also adressed in this part.

2. Theory

Subject to our theory is the coupled electron-phonon system in an external electric field $\bar{F}$. The one electron potential consists of the periodic lattice part $V_o(\bar{x})$, the trap potential $V_t(\bar{x})$, the electron-phonon interaction $V_{ep}(\bar{x},Q)$, and the potential $-e\bar{F}\cdot\bar{x}$. H_p is the Hamiltonian of lattice ions. The total wave function of the coupled system, $\Psi_{\lambda N}$, at first, is taken in an approximation where transitions between different electron states caused either by lattice motion or by switching on the electric field are omitted. In a second step these transitions are included by means of time dependent perturbation theory. In the first step we set $\Psi_{\lambda N} = \varphi_\lambda \cdot \phi_{\lambda N}$ with the electron state φ_λ and the lattice state $\phi_{\lambda N}$ given by a certain set of coupled equations. We use the static version of these equations. Its equivalence to the adiabatic version has been demonstrated recently by Peuker et. al. (1982) and Burt (1982) in first order perturbation theory and with the neglect of anharmonicity. The static equations read (with $\hbar$ equal to 1)

$$(-(1/2m_o)\Delta + V_o(\bar{x}) + V_t(\bar{x}) - e\bar{F}\cdot \bar{x}_{diag})\varphi_\lambda = \varepsilon_\lambda \varphi_\lambda \quad (1)$$

$$(H_p + (\varphi_\lambda | H_{ep} | \varphi_\lambda) + \varepsilon_\lambda) \Phi_{\lambda N} = E_{\lambda N} \Phi_{\lambda N} \quad (2)$$

where $\bar{x}_{diag}$ means the diagonal part of $\bar{x}$ with respect to the discrete component of the set of electronic quantum numbers λ, usually being the band or the deep level index. The rate of electron emission, e_n, from deep level states λ into band states λ' caused by phonon and electric field induced transitions is calculated by applying the "Golden Rule"

$$e_n = 2\pi \sum_{\lambda\lambda'} \sum_{NN'} p_n |(\Phi_{\lambda N}\varphi_\lambda | V_{ep} - e\bar{F}\cdot\bar{x} | \varphi_{\lambda'} \Phi_{\lambda' N'})|^2 \delta(E_{\lambda N} - E_{\lambda' N'}). \quad (3)$$

Here p_N means the statistical weight of the lattice initial states, the λ, λ'-summation extends upon occupied electron initial states and empty electron final states. The explicit calculation of electron states is carried out for a two band model with a parabolic and isotropic valence band $E_v(\bar{k})$ having its maximum at $\bar{k} = 0$ (effective mass m_v), and a parabolic ellipsoidal conduction band $E_c(\bar{k})$ having its minimum at $\bar{k}_o$ (effective masses m_l , m_t). We postulate the possibility to build the deep level states only from valence states while the continuum states are assumed to be built only from Bloch functions of the conduction band near $\bar{k}_o$. There are no arguments that these assumptions are completely fulfilled in the case of deep levels under consideration, but there a r e arguments that the main features of theoretical results, to a certain extent, are insensitive to the details of electron states. The envelope equations for them read

$$(E_c(\bar{k} - \bar{k}_o) - E + ie\bar{F}\cdot\nabla_k)\ \varphi_{cE}(\bar{k}) = 0 \quad (4)$$

$$(E_v(\bar{k}) - E + ie\bar{F}\cdot\nabla_k)\varphi_{tE}(\bar{k}) + \sum_{k'} (v\bar{k} \mid V_t \mid v\bar{k}')\varphi_{tE}(\bar{k}') = 0. \quad (5)$$

We restrict ourselves to neutral trap centres. In this case the particular choice of V_t is not essential as long as it produces one bound state in the gap for zero electric field and the wave function of this state is not essential inside the potential well. Taking the pseudo--potential $V_t = V_0\, \delta(\bar{x})\ (1 + \bar{x}\cdot\nabla)$, equation (5) can be solved exactly even in the presence of an electric field /4/. One finds that the deep level is asymmetrically broadened, its maximum of state density is shifted, and its wave function is changed due to the electric field. As long as field strengths are below a certain threshold value (10^6 V/cm in typical cases /4/) these effects are much smaller than the field effect on band states. Here we neglect them completely. At extremely high fields they have to be taken into account. How this can be done was demonstrated in /4/ in the case of optical transitions. For the lattice vibration we use the Einstein model. With these assumptions the emission rate from equ. (3) can be transformed into the closed expression

$$e_n = e^{-S(2\bar{N}+1)} \sum_{l<0} ((\bar{N} + 1)/\bar{N})^{1/2} (c_F F^2 + c_p\ (S - l)^2/S) \times I_l(2S(\bar{N}(\bar{N} + 1))^{1/2})\ D_c(- E_B - l\omega_0) \quad . \quad (6)$$

Here $c_F \sim |(c\bar{k}_0|\bar{x}\cdot\bar{F}/F \mid v\bar{k}_0)|^2$ and $c_p \sim |(c\bar{k}_0| \partial V_{ep}/\partial Q \mid v\bar{k}_0)|^2$, up to a certain constant, are the squared absolute values of the transition matrix elements, ω_0 is the phonon frequency, and S the Huang-Rhys-factor. $E_B = E_g - E_B^0 + S\omega_0$ means the effective trap depth measured from the bottom of the conduction band, $\bar{N}$ is the Bose function an I_l the modified Bessel function for integer l. $D_c(E)$ denotes the conduction band density of states in the presence of an electric field,

$$D_c(E) = 1/2\pi^2\ (8m_{\parallel}\, m_{\perp}^2)^{1/2}\ \theta^{1/2}\ (Ai'^2(- \tfrac{E}{\theta}) + \tfrac{E}{\theta}\ Ai^2(- \tfrac{E}{\theta})), \quad (7)$$

$$m^{-1}_{\parallel,\perp} = (m^{-1}_{t,l}(\bar{k}_0 \times \bar{F}) + m^{-1}_{l,t}\ (\bar{k}_0\cdot\bar{F}))/k_0 F \quad , \quad \theta = ((eF)^2/2m_{\parallel})^{1/3} \quad (8)$$

with Ai as the Airy-function. The assumption $m_v \gg m_{\parallel}$ has been made in de-

riving expressions (6), (7). The emission rate (6) describes, in a unified way, phonon assisted tunneling and tunneling enhanced multiphonon transitions. The two processes are vizualized by the configuration coordinate diagram of electron states in fig.1. Decreasing line thickness in the drawing means decaying field induced density of states within the gap. Expression (6) accounts only for emission to o n e valley of the conduction band. To get the total rate one has to sum upon all valleys. For small field strength and final state energies $E < 0$ within the gap $D_c(E)$ transforms asymptotically into the well-known WKB expression $\sim(F/E) \cdot \exp(-(4m_{\parallel} E^3)^{1/3}/3eF)$ for the tunneling probability through a triangular barrier. This asymptotic expression fails for energies close to the conduction band edge. Using it would lead to an overestimation of tunneling in this energy region and would produce a serious error in e_n at higher temperatures. Thus the exact expression (7) has to be taken.

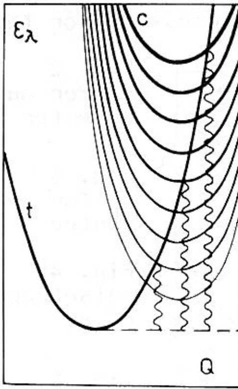


Fig.1 Multiphonon transitions in an electric field

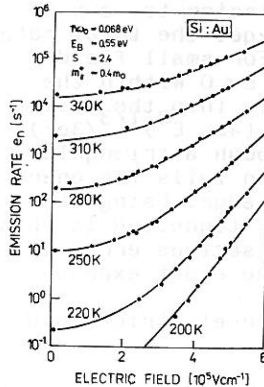
3. Experimental

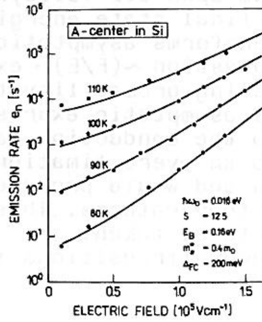
Samples were prepared from Czochralski-grown [111] -oriented n-type silicon. Wafers of various resistivities were gold diffused at temperatures of about 1000°C and then chemically etched to form samples with homogenous gold distribution. For the generation of radiation damage, defect ion implantation was used. The implantation energy and dose of protons or helium ions were choosen so that the defect distribution was accessible for the analysis by capacitive methods and that the maximum deep level concentration was below the shallow doping density. Schottky diodes were fabricated by vacuum evaporation of gold. The deep level properties were measured by means of a special DLTS spectrometer based on a modified lock-in filtering method allowing double correlation DDLTS as suggested by Lefevre and Schulz (1977). In this way it was possible to get carrier emission signals of a particular deep level from a small spatial window of the whole space charge region. The width of the window was choosen small enough to be sure that the electric field strength was constant within 10%. For an exact evaluation of the depth we used capacitance-voltage measurements at the relevant temperatures. The results were corrected by taking into account their dependence on the pulse width in relation to the capture rate of the deep level. Only samples with constant net donor concentrations were investigated. So the dependence of the electric field on the depth in the space charge region was linear. The two possibilities of varying the electric field strength - first, changing the position of the spatial window at fixed reserve bias and second, changing the reverse bias while keeping fixed the spatial window - yielded consistent results (confirming the field strength evaluation). The measurements were performed by choosing a constant emission rate window and registering the temperature shift of the DDLTS peak as a function of the electric field. By interpolating of these data the electron emission rate could be obtained as a function of the electric field with the temperature as parameter.

4. Results and Discussion

Two neutral centres were investigated experimentally, first the Au-related acceptor, and second the A-centre usually related to the vacancy-oxygen-complex. The experimental results for the emission rates are plotted in fig 2 and 3 together with theoretical curves calculated from expression (6). The electric field is parallel to [111] . For this field

direction all valleys are equivalent. In the case of the Au-acceptor the following commonly accepted parameters are used /5/: ω_o = 0.068 eV, S = 2.4, E_B = 0.55 eV. This choice deviates from the one in /3/ where unusual values had to be taken to get agreement with an approximate version of the theory from /1/. The value of the effective mass $m_{\parallel}$ necessary for the





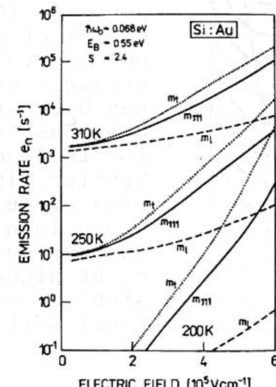
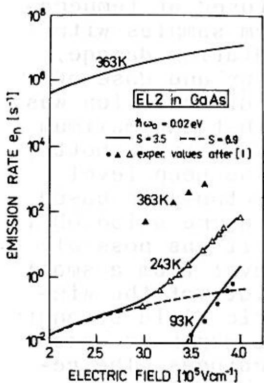


Fig. 2 e_n for Au-acceptor

Fig. 3 e_n for A-centre

Fig. 4 Anisotropy of e_n

Fig. 5 e_n for EL2-centre



best fit is $m_{\parallel}$ = $0.4m_o$. It deviates from the true conduction band mass in [111] -direction which amounts $0.26m_o$. This discrepancy results from the simplifying assumption of a parabolic conduction band structure which does not apply to $\bar{k}$-space regions more distant from $\bar{k}_o$. Since essential contributions to the emission rate arise also from these regions, a $\bar{k}$-space average of $m_{\parallel}$ has to be expected instead of the true value $m_{\parallel}$. In general, the field dependence of the emission rate is very sensitive to the effective mass $m_{\parallel}$. This leads to a remarkable anisotropy of the field effect of electron emission in silicon. Fig.4 shows this anisotropy for the Au-acceptor according to our theory. In fig.3 we compare experimental and theoretical results for the A-centre. The same effective mass $m_{\parallel}$ = $0.4m_o$ has been used as before in the case of the Au-acceptor. From /3/ we take E_B=0.155 eV. Then ω_o = 0.016 eV and S=12.5 give the best fit to the experimental results. Our theory can be also applied to the EL2 centre in GaAs. In fig. 5 we show experimental data from /1/ together with our calculated curves. For low temperatures we can achieve good agreement with ω_o=0.02 eV and S=3.5. The same parameters do not fit experimental data at higher temperatures (see fig.5). With S=6.9 as reported in /1/, we were not able to achieve a reasonable fit at any temperature. One possibility to explain these discrepancies would be the assumption of a second phonon mode which contributes to the emission rate at higher temperatures. The observed strong anisotropy of the field effect for the EL2 centre /6/ cannot be explained by an effective mass anisotropy like the one observed in silicon. The results in /6/ seem to indicate a more complex, anisotropic structure of the EL2 centre.

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