(Mo-P-15) ELECTROABSORPTION AT DEEP CENTRES ACCOMPANIED BY MULTIPHONON PROCESSES*

By A. Schenk, R. Enderlein and D. Suisky

Humboldt-Universität zu Berlin, Sektion Physik**

(Received August 7, 1985)

The electroabsorption spectrum for transitions from a deep impurity level to the conduction band is calculated in the framework of the Lucovsky model. Effects of multiphonon processes due to the strong lattice coupling are taken into account. The line shape turns out to be highly susceptible to the ratio of electrooptical and phonon energy.

PACS numbers: 78.50.Ge

1. Introduction

Although the description of the electronic structure of deep defects and impurities without any external perturbation has been improved by self-consistent Green's-function methods during the last years, one needs in addition the non-perturbation results for the wave functions to get the field and temperature dependent transition probabilities, if radiative or non-radiative recombination processes in an electric field are considered. Among the experimental methods developed for determination of the defect nature, wave functions, binding energies, cross sections and other properties, the optical techniques play an important role. Thus it is useful to study both the essential influence of a strong electric field and of multiphonon excitation and deexcitation processes on the optical transitions from impurity to band states. The complexity of this problem can be reduced by adopting a 3-dimensional δ-potential model which allows the exact analytical solubility even in the presence of an electric field [1]. In [1] the zero phonon absorption spectrum has been calculated for transitions from the impurity level to the band from which the level splits up. The same model has been applied to the case of transitions from valence band to impurity states accompanied by multiphonon processes in [2]. As long as the field strengths are below a certain threshold value (10^6 V/cm in typical cases) the field effects on localized states are much smaller than those on band states and can be neglected. We will follow

* Proc. XIV School on Physics of Semiconducting Compounds, Jaszowiec 1985.

** Address: Humboldt-Universität zu Berlin, PSF 1297-1086 Berlin, GDR.

this approach regarding the well known Franz-Keldysh-effect on band states [3] to be responsible for the characteristic line shape of the field-induced change in the absorption coefficient.

2. Theory

Optical transitions from deep level states λ into the band states λ' which are assumed to be dipole allowed are calculated by applying the "Golden Rule". The result for the absorption coefficient is (cf. [4])

$$\alpha(\omega, \vec{F}) = \frac{C}{\omega} \sum_{\lambda\lambda'} \sum_{NN'} p_N |(\phi_{\lambda' N'} \varphi_{\lambda'} | \vec{\varepsilon} \cdot \vec{\nabla} | \varphi_\lambda \phi_{\lambda N})|^2 \delta(E_{\lambda' N'} - E_{\lambda N} - \hbar\omega). \tag{1}$$

In (1) φ and ϕ are the electronic and vibronic eigenstates of the coupled electron-phonon system, $\vec{\varepsilon}$ denotes the polarisation vector of the radiation and 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. In the following we will neglect both the electron-phonon coupling for final states and the field influence on localized initial states ($\vec{F}$ — electric field strength). Consequently the field dependence of $\alpha(\omega, \vec{F})$ is only due to the band states $\varphi_{\lambda'}$. The explicit calculation of electron states is carried out for a two band model with a parabolic and isotropic valence band $E_v(\vec{k})$ (effective mass m_v) and a parabolic ellipsoidal conduction band $E_c(\vec{k})$ (effective masses m_l, m_t). We consider only direct transitions and 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 $\vec{k} = 0$. This approach should be reasonable for deep neutral centres attached to the valence band. The set of Schrödinger equations for the two envelope wave funotions reads (neglecting the interband transitions and the intraband polarisation of the Bloch functions)

$$[E_c(\vec{k}) - E + ie\vec{F} \cdot \vec{\nabla}_{\vec{k}}] A_E^c(\vec{k}) = 0, \tag{2.1}$$

$$[E_v(\vec{k}) - E] A_E^t(\vec{k}) + \sum_{\vec{k}'} (v\vec{k} | V_t(\vec{x}) | v\vec{k}') A_E^t(\vec{k}') = 0, \tag{2.2}$$

where

$$V_t(\vec{x}) = V_0 \delta(\vec{x}) [1 + \vec{x} \cdot \vec{\nabla}_{\vec{x}}] \tag{3}$$

is the defect potential taken after Vinogradov [1]. As has been shown in [5] a δ-potential gives good results for the energy dependence of zero field optical cross sections, which justifies its use in our calculation. Equation (2.2) results in one bound state in the gap at an energy $E = -E_g + E_B^0$, if $V_0 = 4\pi E_B^0 r_0^3$ (r_0 — localisation radius $r_0^2 = \hbar^2/2m_v E_B^0$). We obtain from (2)

$$D_c(E) = |A_E^c(0)|^2 = \frac{1}{4\pi\hbar^3} \sqrt{8 m_\parallel m_\perp m_t} \sqrt{\hbar\theta_\parallel}\, \mathcal{F}\left(-\frac{E}{\hbar\theta_\parallel}\right), \tag{4.1}$$

$$D_t(E) = |A_E^t(0)|^2 = (2\pi r_0^3)^{-1} \delta(E + E_g - E_B^0), \tag{4.2}$$

the quantities needed for the calculation of the total electronic transition rate $D(E', E)$ for a transition $E \to E'$. The expression (4.1) describes the well known Franz–Keldysh tails below and the oscillations around the zero field threshold. ($\mathscr{F}(y) = Ai^2(y) - yAi^2(y)$; $\hbar\theta_{||} = \left(\frac{(e\hbar F)^2}{2m_{||}}\right)^{1/3}$ — electrooptical energy; $1/m_{||,\perp} = \sin^2\vartheta/m_{t,l} + \cos^2\vartheta/m_{l,t}$; ϑ — angle between the electric field and the rotational axis of the energy ellipsoid). The total transition rate $D(E', E)$ can be expressed in form of a simple product:

$$D(E', E) = \frac{V_0^2}{\left(E + E_g + \frac{m_\perp}{m_v} E'\right)^2} D_l(E) D_c(E') . \tag{5}$$

Using Eqs (1), (4) and (5) and $(ck'|\vec{\nabla}|vk) \approx (i/\hbar)\vec{p}_{cv}(0)\delta_{\vec{k}\vec{k}'}$ the field dependent absorption coefficient can be written as

$$\alpha(\omega, F) = \frac{C|\vec{\varepsilon} \cdot p_{cv}|^2}{\omega\hbar^2} \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} dE' D(E', E) I_{E'E}(\omega), \tag{6}$$

where $I_{E'E}(\omega)$ is the Fourier transform of the lineshape function known from the multiphonon theory [6]. Restricting to one effective phonon energy $\hbar\omega_0$ and using the asymptotic behaviour of $\mathscr{F}(y)$

$$\lim_{\vec{F}\to 0} \mathscr{F}(y) = \frac{1}{\pi}\theta(-y)\sqrt{-y}$$

the field induced change in $\alpha(\omega)$ can finally be transformed into a sum of thermally weighted electro-optical functions of the first kind $F(y) = \pi\mathscr{F}(y) - \theta(-y)\sqrt{-y}$

$$\Delta\alpha(\omega) = \alpha_0 e^{-S(2\bar{N}+1)} \sum_{l=-\infty}^{\infty} \left(\frac{\bar{N}+1}{\bar{N}}\right)^{l/2} I_l(2S\sqrt{\bar{N}(\bar{N}+1)})$$

$$\times \frac{\sqrt{\hbar\theta_{||}}\, F[(E_B + l\hbar\omega_0 - \hbar\omega)(\hbar\theta_{||})^{-1}]}{\omega\left[E_B^0 - \frac{m_\perp}{m_v}(E_B + l\hbar\omega_0 - \hbar\omega)\right]^2} . \tag{7}$$

In our final expression (7) I_l denotes the modified Bessel function of order l and E_B means the effective trap depth measured from the bottom of the conduction band: $E_B = E_g - E_B^0 + S\hbar\omega_0$. ($\bar{N}$ — Bose occupation number, S — Huang-Rhys factor).

3. *Numerical results*

In figures 1a-d we have plotted the line shapes at $T = 10$ K for various field strengths and Huang–Rhys factors using equation (7). The zero phonon line indicated in each figure exhibits a pure shape of the electrooptical function F, slightly modified by the energy denom-

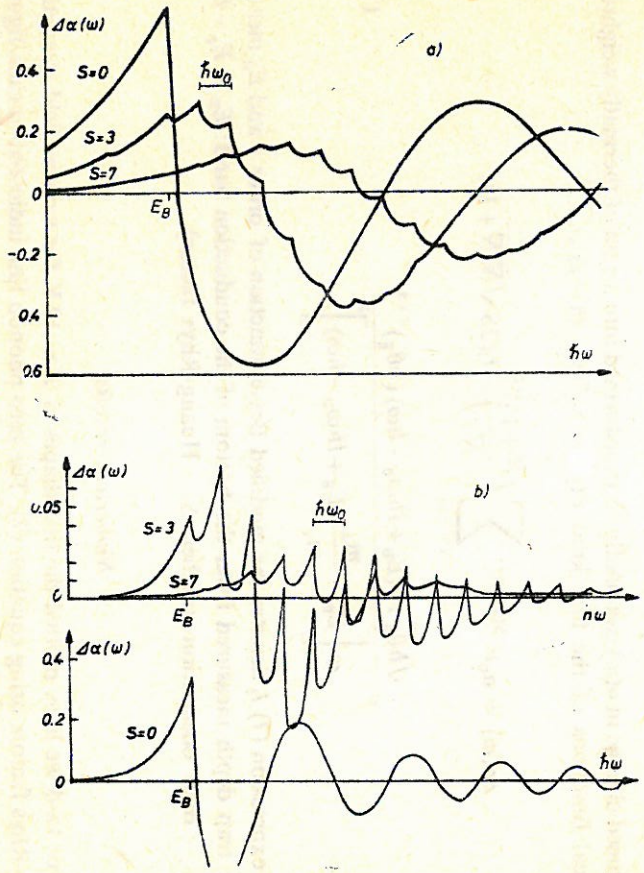

Fig. 1a, b

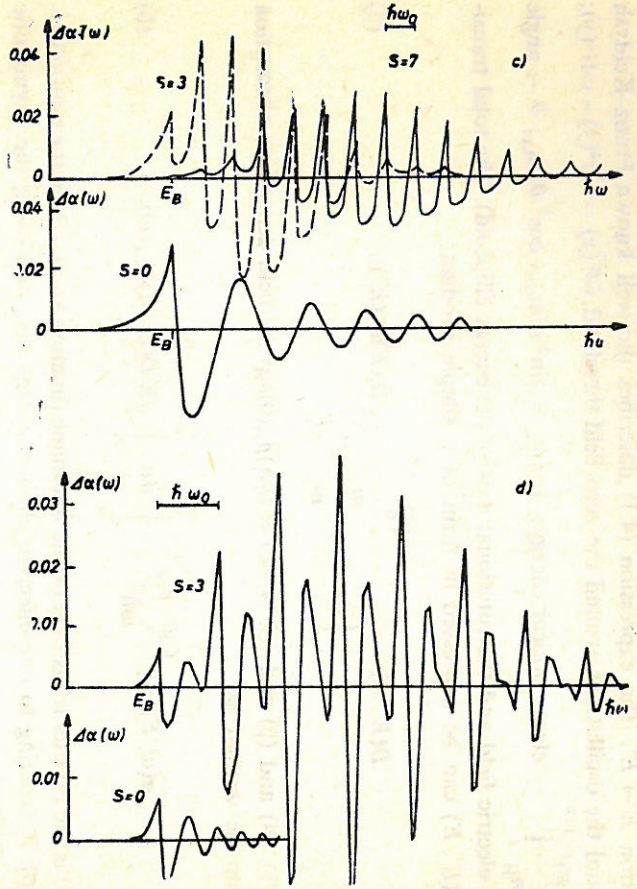

Fig. 1c, d

Fig. 1a. Electroabsorption spectrum $\Delta\alpha(\omega)$ for different Huang–Rhys factors: $S = 0\,(1), S = 3\,(2), S = 7\,(3)$. The following parameters have been used: $\hbar\theta_{||} = 113$ meV, $\hbar\omega_0 = 20$ meV, $E_B/\hbar\omega_0 = 30$, $T = 10$ K. The energy scale is in units of the effective phonon energy $\hbar\omega_0$. E_B denotes the trap depth. b. Same key as figure 1a, but for $\hbar\theta_{||} = 39$ meV. c. Same key as figure 1a, but for $\hbar\theta_{||} = 24$ meV. d. Same key as figure 1a, but for $\hbar\theta_{||} = 5$ meV

minator in (7). For high fields the line shape is determined by F, which gets increasingly broadened with rising coupling strengths and the first zero value of which turns out to be shifted by the Franck–Condon energy $S\hbar\omega_0$ (figure 1a).

The discrete nature of the spectrum due to the Einstein model, which is only weak for large field strengths, becomes dominant in the case of lower fields. Below a certain electrooptical energy, when the first oscillation of F has an energetic distance less than the effective phonon energy, additional substructures arise (figure 1d). The height of the peaks can grow with decreasing fields now, depending on whether a maximum of F coincides with $\hbar\omega_0$ or not.

REFERENCES

[1] V. S. Vinogradov, *Fiz. Tverd. Tela* **13**, 3266 (1971).

[2] R. Enderlein, D. Fiddicke, F. Bechstedt, K. Peuker, R. S. Bauer, Luminescence Conference, Berlin (West) 1981.

[3] A. Schenk, K. Irmscher, D. Suisky, R. Enderlein, F. Bechstedt, H. Klose, 17th Intern. Conf. Phys. Semicond., San Francisco 1984.

[4] A. Schenk, R. Enderlein, D. Suisky, *Phys. Status Solidi.* (b) **131**, 729 (1985).

[5] G. Lucovsky, *Solid State Commun.* **3**, 299 (1965).

[6] K. Huang, A. Rhys, *Proc. Roy. Soc.* **A204**, 406 (1960).