(Mo-P-37) DETERMINATION OF DEEP CENTRE PARAMETERS FROM ELECTROABSORPTION SPECTRA*

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(Received June 2, 1987)

A theory is developed for the electric-field induced changes of optical absorption spectra due to multiphonon-assisted transitions from deep level into band states. The theory can be used for the determination of deep centre parameters.

PACS numbers: 71.55.–i, 78.20.Jq, 78.50.Ge

1. Introduction

Deep centre and band structure parameters of doped and undoped semiconductors have been obtained by different experimental techniques based on optical, electrical, mechanical and magnetical effects or a combination of them, e.g. electrooptical, magnetooptical and piezooptical effects [1]. All these techniques have been developed for studying bulk crystals but they can be also used for the investigations of superlattices [2]. One type of measurements which allows one to determine band parameters as well as deep-centre parameters with high accuracy is the electroabsorption (EA) technique. Usually the electric field strength varies from 1×10^4 V/cm up to a few 10^5 V/cm and the EA spectra of interband transitions are known to be of rich structure. The change of the absorption coefficient is induced by the mixing of different electronic states due to the presence of the electric field causing characteristic oscillations with photon energy (Franz-Keldysh effect [3]). The typical parameter on which the line-shape depends is the electrooptical energy $\hbar\theta_{\|} = (e^2\hbar^2F^2/2m_{\|})^{1/3}$ (F electric field strength, $m_{\|}$ effective mass in field direction). For low field strengths, life-time broadening may be important if the relation $\hbar\theta_{\|} \ll \Gamma$ is fulfilled. Then the EA spectrum can be represented as the third derivative of the absorption spectrum (low field limit). EA techniques have been also employed for studying intra-centre transition between localized gap states [4, 5] by using the electric-field induced

* Proc. XVI School on Physics of Semiconducting Compounds, Jaszowiec 1987.

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shift of the electronic levels due to the Stark effect. In this case, theory predicts an EA signal of the first derivative type instead of the third-derivative type in the case of interband transitions. The energetic width of the spectrum of intracentre transitions is determined by the strength of the electron-phonon interaction. Thus, the spectrum turns out to be the broader the stronger the electron-phonon coupling is. The EA spectrum is relatively smooth [5] in contrast to the case where transitions take place from band to band states. In the case of transitions between band and localized states one expects a combination of the two characteristic features mentioned above. The EA lineshape should depend both on the electrooptical energy $\hbar\omega_{\mathrm{ph}}$ as well as on the electrooptical energy $\hbar\theta$.

In this paper we will treat the intermediate type of transitions (band to centre), where all of the typical energies, $\hbar\theta$, Γ and $\hbar\omega_{\mathrm{ph}}$, came into play and determine together the lineshape of the EA spectrum.

2. *Theory*

We study the influence, both of the strong electric field and of the multiphonon excitation and deexcitation processes on the dipole allowed optical transitions from deep centre to band states. The complexity of the problem can be reduced by adopting a 3-dimensional δ-potential model which allows an exact analytical solution to be obtained even in the presence of an electric field [6, 7]. In [6] the zero-phonon absorption spectrum has been calculated for transitions from an impurity level to 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 [7]. As long as the field strengths are below a certain threshold value (10^6 V/cm in typical cases) the field effect on the localized initial states is much smaller than that on the final band states and can be neglected, i.e. the Stark effect can be neglected in comparison to the Franz-Keldysh effect. The lineshape is determined by the Franz-Keldysh oscillations. As it has been demonstrated in [8] the field-induced change of the absorption coefficient is:

$$\alpha(\omega) = \alpha_0 e^{-S(2\bar{N}+1)} \sum_{l=-\infty}^{\infty} \left(\frac{\bar{N}+1}{\bar{N}}\right)^{1/2} I_l(2S\sqrt{\bar{N}(\bar{N}+1)}) \times \frac{\hbar\theta F[(E_{\mathrm{B}}+l\hbar\omega_{\mathrm{ph}}-\hbar\omega)(\hbar\theta_{\parallel})^{-1}]}{\omega\left[E_{\mathrm{B}}^0 - \frac{m}{m_v}(E_{\mathrm{B}}+l\hbar\omega_{\mathrm{ph}}-\hbar\omega)\right]^2}. \tag{1}$$

E_{B} means the effective trap depth measured from the bottom of the conduction band. $E_{\mathrm{B}} = E_{\mathrm{g}} + S\hbar\omega_{\mathrm{ph}}$. I_l denotes the modified Bessel function of order l. S is the Huang-Rhys factor. $\bar{N}$ is the mean occupation number of phonon states. $F(y)$ is the electrooptical function of the first kind [1, 8, 9]. Equation (1) can be used for the calculation of the lineshape of $\alpha(\omega)$ depending on the ratio of $\hbar\theta_{\parallel}$ and $\hbar\omega_{\mathrm{ph}}$ which has been reported in [8].

3. Comparison with experiment. Determination of deep centre parameters

Sokolov et al. [10, 11] have measured the EA spectrum of ZnSe doped with Ni. They have found two groups of positive and negative EA peaks, one around 1.85 eV and one around 2.64 eV. The latter group of structures has been attributed to a transition of an electron from the $^3T_1$ state of the Ni^{2+}-ion (d^8 configuration) slightly above the valence band to the conduction band edge, leaving behind an Ni^{3+}-ion in its ground state to which the electron is bound by Coulomb forces [11]. The change of absorption has been assumed to be caused by the excitonic features of this transition. There is a second possibility for the mechanism responsible for the electric-field induced change of the absorption coefficient, the half-sided Franz-Keldysh effect. This mechanism, accompanied by multiphonon processes, has been discussed in general terms in [8]. Here, we apply the general results to the experimental situation studied by Sokolov et al. [10]. The measurements are performed at low temperatures ($T = 4.2$ K and 77 K). The 4.2 K spectrum is of rich structure and all the information we are interested in can be deduced from it. The position of the first maximum is equal to thermal binding energy $E_B = E_g - 2.637$ eV. From the oscillation width one obtains the electrooptic energy $\hbar\theta_{||} = 3.5$ meV. The difference between the energetic positions of the maximal positive amplitudes is identical with the effective phonon energy $\hbar\omega_{ph} = 22.1$ meV. From the maximum of the envelope function, $E = E_B + S\hbar\omega_{ph}$, it is possible to obtain the value of the Huang-Rhys factor $S = 3.5$. This procedure is confirmed by comparing the 4.2 K and the 77 K spectral line-shapes. The maxima of the envelope function are found to be in good agreement.

Furthermore, all the main peaks of the experimental spectrum can be assigned by applying the theory and assuming the approximations discussed above. The differences between the theoretical and experimental curves are caused due to the neglecting of broaden-

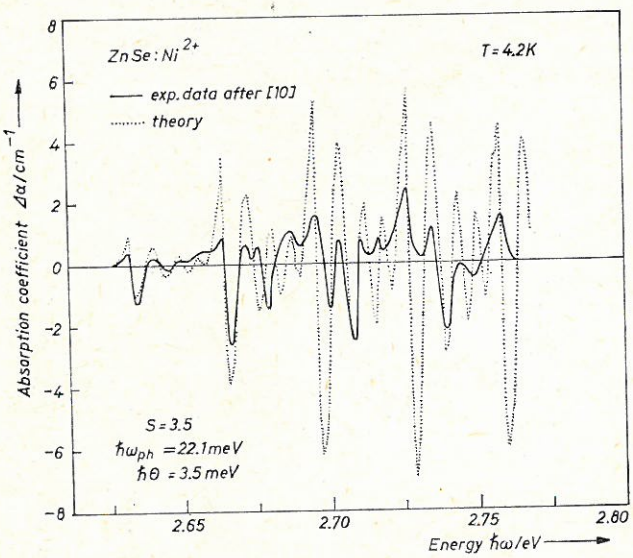

Fig. 1. Electroabsorption spectrum $\alpha(\omega)$ of ZnSe : Ni^{2+}. Experimental data after Sokolov et al. [10]

ing effects (the amplitude should be reduced by life time broadening [1]) and due to the simplification of the degenerate real energy band structure at the top of the valence band. Furthermore, in the energy region $E > E_B + \Delta_{FC}$ one has to expect a superposition of the impurity spectrum and the tail of the conduction band ($E_g = 2.8$ eV).

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