Journal of Luminescence 40&41 (1988) 597–598
North-Holland, Amsterdam

DETERMINATION OF DEEP CENTRE PARAMETERS FROM ELECTROABSORPTION SPECTRA

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

Humboldt-Universitaet zu Berlin, Sektion Physik, 1040 Berlin, Invalidenstrasse 110, GDR

A theory is presented for the electric field induced changes of optical absorption spectra due to multiphonon assisted transitions from deep level into band states. The electroabsorption line shape is determined by an interplay between the final state Franz-Keldysh oscillations and the multiphonon oscillations. It is demonstrated that deep centre parameters can be derived with high accuracy from experimental electroabsorption spectra.

1. INTRODUCTION

The appreciable changes of optical absorption due to an external electric field make electroabsorption (EA) a powerful tool for the investigation of energy bands and deep levels in semiconductors and insulators. Most of the previous work on EA involving deep levels has been devoted to the case of intra-centre transitions. The linear and the quadratic Stark shifts of the deep levels are responsible for the field induced changes of absorption in this case, and the EA line shapes are given by, respectively, the first and the second derivatives of the zero field absorption spectra. Much less work exists on EA in the case of transitions from deep levels into bands, or, vice versa , bands into deep levels. The existing experimental investigations[1] demonstrate that sharply structured spectra can be obtained under certain conditions which in principle could be used for the determination of characteristic parameters of deep levels, bands and lattice modes. The present paper provides the theoretical basis for this purpose. It extends earlier results by the same authors[2].

2. THEORY

In paper[2] we have theoretically studied the combined effect of multiphonon excitation and deexcitation processes on dipole allowed optical transitions from deep centre to band states. The deep centre has been treated within the Lucovsky δ-potential model which is known to predict reasonable absorption spectra in the case of zero phonon coupling and zero electric field. The application of the Lucovsky model may also be justified in the more complex case of non-zero phonon coupling and non-zero electric field. Here one first faces the problem of treating the electron-phonon coupling in an appropriate way. In our approach this is done by means of the standard theory of multiphonon processes. The Schroedinger equation for the electron wavefunction is rigorously solved in the presence of an electric field. The latter need to be considered only in the final (conduction band) state whereas it can be neglected in the initial (deep level) state. This approximation breaks down only at relatively high electric fields, typically 10^6 V/cm. The lattice vibrations are taken within the Einstein model. The electroabsorption coefficient $\Delta\alpha(\omega,S,F) = \alpha(\omega,S,F) - \alpha(\omega,S,F=0)$ in dependence on photon energy $\hbar\omega$, Huang-Rhys factor S, and electric field strength F may be expressed by means of the electroabsorption coefficient $\Delta\alpha(\omega,F)$ without phonon coupling by taking the weighted sum

0022-2313/88/$03.50

upon all numbers of excited and deexcited phonons in the optical transition: (1)

$$\Delta\alpha(\omega,S,F)=\sum_{l=-\infty}^{\infty}\Delta\alpha(\omega-l\omega_o,F)e^{-S(2N+1)}\sqrt{\frac{N+1}{2}}I_l(2S\sqrt{N(N+1)})$$

Here $\hbar\omega_o$ means the effective phonon energy, N is the average phonon number and I_l the modified Bessel function of order 1. For $\Delta\alpha(\omega,F)$ one has

$$\Delta\alpha(\omega-l\omega_o,F) = f\frac{\sqrt{\theta}\,F((E_t-\hbar\omega+l\hbar\omega_o)/\hbar\theta)}{\omega\{E_B^o-(m_c/m_v)(E_t-\hbar\omega+l\hbar\omega_o)\}^2} \quad (2)$$

where f denotes a certain ω- and F-independent constant, $\hbar\theta=((eF)^2/2m_c\hbar)^{1/3}$ the electrooptic energy, E_B^o the deep centre binding energy, $E_t=E_g-E_B+S\hbar\omega_o$ the effective deep level energy (related to the top of the valence band), and $m_{c/v}$ the conduction and valence band masses, respectively. The electrooptic function F(x) may be expressed in terms of the Airy-function Ai(x) . The field effect on the absorption coefficient as described by the expressions (1),(2) may be characterized as final state Franz-Keldysh (FK) effect. Analogous results are obtained in the case of the optical excitation of holes from the deep level into the valence band.

3. DISCUSSION AND COMPARISON WITH EXPERIMENT

The fine structure of the EA-spectrum (1),(2) is determined by the interplay of the FK-oscillations of period $\simeq\theta$ and the multiphonon oscillations of period ω_o. The EA-line shape depends critically on the ratio θ/ω_o. The interference between the two periodic substructures may result in a decreas of a certain EA-peak with raising F. In the case of high temperatures and /or strong electric fields ($\omega_o \ll \theta\sqrt{2N+1}$) the EA-line shape resembles the well-known EA-spectrum without phonon coupling, the latter being Franck-Condon shifted and Gauss broadened. In the case of low electric fields ($\theta \ll 2\Gamma, \Gamma=\omega_o\sqrt{S(2N+1)}$) the EA-line shape is given by the third derivative of the zero field spectrum. At low temperatures ($N \ll 1$) this results in sharp periodic phonon

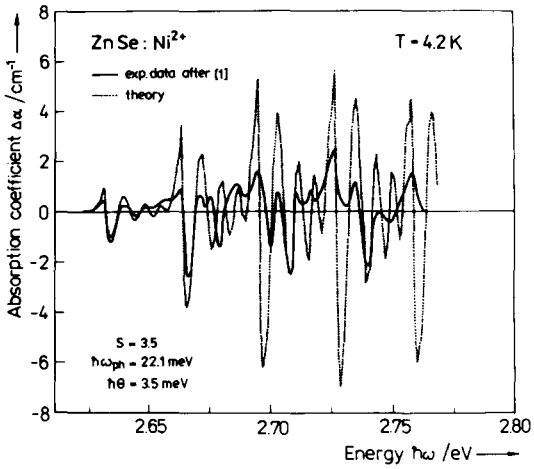

FIGURE 1

Experimental[1] and theoretical low field EA-spectra for ZnSe:Ni

structures which are modulated by a certain envelope function having its maximum at $E_t+S\hbar\omega_o$. Characteristic parameters can be extracted from experimental EA-spectra for all field strengths and temperatures. The low field and low temperature case seems to be the most suitable one. We use experimental data by Sokolov et.al[1] for ZnSe:Ni taken at 4.2K as an example.e The EA-structure around 2.7eV is attributed to a transition of an electron from the $^3T_1$ state of the Ni^{2+}-ion into the conduction band. The position of the first maximum gives the deep level energy E_t=2.637eV. The oscillation width yields $\hbar\theta$=3.5meV, the distance between the main maxima $\hbar\omega_o$=22.1meV, and the maximum of the envelope function S=3.5.

References

1. V.I. Sokolov, T.P. Surkova, V.V. Chernyaev, phys. stat. sol.(b) 144 (1982) K 195

2. A. Schenk, R. Enderlein, D. Suisky, phys. stat. sol.(b) 131 (1985) 729