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Optical Absorption in GaSe and GaS

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(13.V.64)

Abstract. A model is proposed to account for some of the optical properties of GaSe and GaS. The dependence of the absorption in the neighbourhood of the edge upon the orientation of the polarisation vector of the incident radiation can then be accounted for. In addition, the transition in GaS is shown to be indirect and forbidden.

GaSe and GaS are made up of isomorphous four-fold layers in which the Se and S atoms occupy equivalent sites, and the structures differ only in the manner in which the layers are stacked[1]). Since the bonding within a layer is predominantly covalent with a small ionic contribution whereas that between layers is of the van der Waals type, the band schemes of GaSe and GaS are likely to be similar.

The following model is proposed to account for some of the optical properties of the compounds. Free charge-carriers occurring within one layer are considered as being confined to that layer. In other words the crystal properties are to be determined from consideration of a single isolated layer. The potential affecting the charge carriers is written as a sum of two parts. The first describes the potential in the z-direction normal to the layers and is taken to be a one-dimensional potential well. The second part describes a potential periodic in x and y in the plane of the layers. The electron wave functions are then written as

$$\Psi_{p\,q\,\underset{\sim}{k}}(x, y, z) = S_{p\underset{\sim}{k}}(x, y)\; Z_q(z)\;. \tag{1}$$

The $S_{p\underset{\sim}{k}}$ are solutions of a two-dimensional Schrödinger equation containing the periodic potential; the Z_q are wave functions of an electron in a one-dimensional potential well. The resultant energy band scheme is then described by a series of levels corresponding to the Z_q each of which is associated with a two-dimensional band representation corresponding to the $S_{p\underset{\sim}{k}}$. The situation is represented schematically in Figure 1 which shows the density of states as a function of energy. In order to account for the semiconducting behaviour an energy gap is introduced in the two-dimensional S-band scheme.

Two possible optical transitions are shown in Figure 1. In transition 1 an electron is excited from one of the S-bands associated with a given Z-level to a different S-band associated with a second Z-level. In transition 2, an electron is excited from one S-band to a second S-band across the energy gap in the two-dimensional band scheme, both

bands being associated with the same Z-level. On the basis of the model we cannot deduce which transition occurs at lower energy. Experiments described below lead us to believe that in GaSe and GaS the absorption edge arises from transition 1.

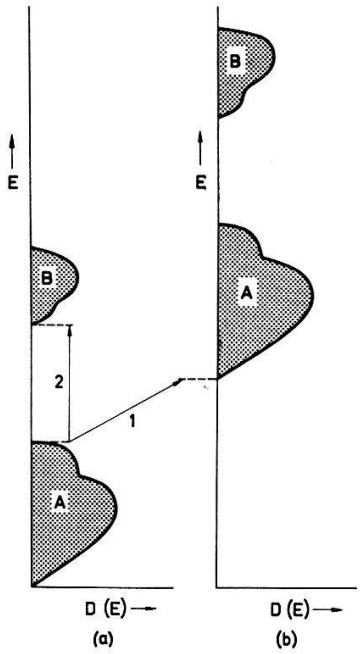

Figure 1

Schematic representation of the density of states of the band system of GaSe and GaS. The S-bands A and B on the left hand side of the figure are associated with Z_0, the same bands on the right hand side with Z_1. In transition 1 both the S- and Z-functions change. In transition 2 only the S-functions change.

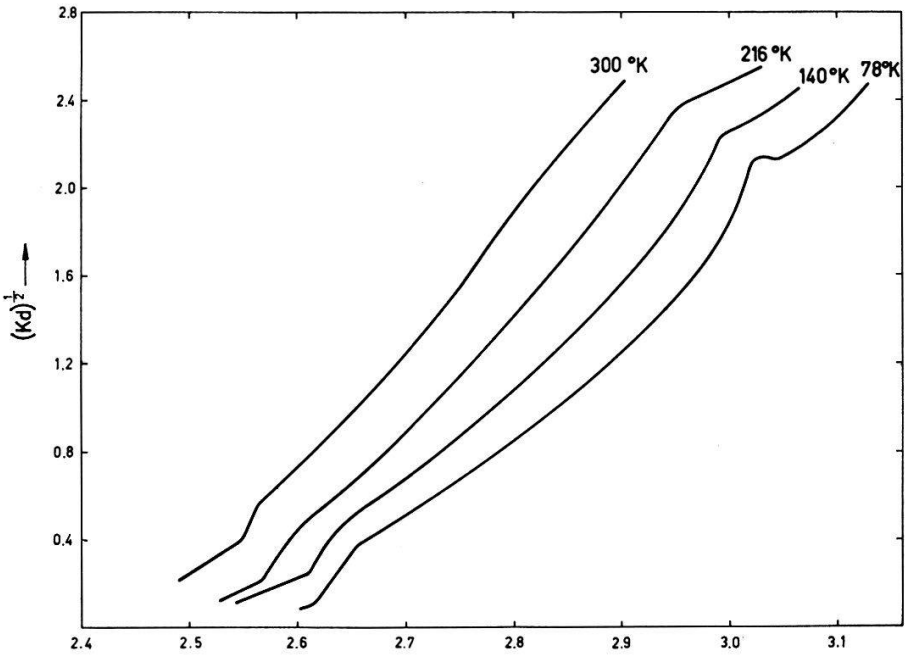

Figure 2

The square root of the absorption coefficient of pure GaS between 300° K and 78° K as a function of energy.

For allowed optical transitions the energy dependence of the absorption coefficient arises from variation with energy of the density of states of the valence and conduction bands; in our case the variation arises from the S-bands only. If the bands are assumed to be isotropic in x and y and quadratic in $\underset{\sim}{k}$ it is found that an indirect transition gives rise to a linear relationship between the absorption coefficient and the photon energy whereas a direct transition leads to a step-function, i.e.

$$K_{direct} \quad \text{independent of } h\nu\text{; step-function,}$$

$$K_{indirect} \quad \alpha(h\nu - \Delta E \pm E_p) .$$

When the transition is forbidden we have

$$K_{direct} \quad \alpha(h\nu - \Delta E) ,$$

$$K_{indirect} \quad \alpha(h\nu - \Delta E \pm E_p)^2 .$$

Figure 2 shows the absorption of a thick sample of GaS between 300° K and 77° K for unpolarised radiation at normal incidence. The absorption tail extends over several tenths of an electron volt and the slope decreases as the temperature decreases. Further evidence of the participation of phonons in the absorption is provided by the abrupt increases in absorption immediately after the onset. These are interpreted as being due to phonon emission. The mean separation of the increases from the onset of absorption at different temperatures leads to a value of 420 °K for the phonon, assuming only one type to be dominant. The nearest approach to a straight line is obtained by plotting $(K\,d)^{\frac{1}{2}}$ versus the phonon energy, where d is the sample thickness, in this case 65 μ. Following the discussion of absorption given above we conclude that the transition is indirect and forbidden in GaS and direct and forbidden in GaSe.

The absorption of both GaSe and GaS was found to depend markedly on the polarisation of the radiation when incident at 45°. With the polarisation vector parallel to the plane of incidence the absorption was found to increase by an order of magnitude over that with polarisation vector normal to the plane. The increase becomes greater at higher angles of incidence and it is assumed that the absorption is in fact a maximum when the polarisation vector is parallel to z.

The probability of a transition from a state with wavefunction Ψ_i to a state with wavefunction Ψ_f is governed by the square of the matrix element

$$\int \Psi_f^* \, H \, \Psi_i \, d\tau$$

where $H = -\,i\,e\,\hbar/m\,c\,\underset{\sim}{A} \cdot \mathrm{grad}$; $\underset{\sim}{A}$ is the vector potential characterising the radiation. When $\underset{\sim}{A}$ is parallel to z the transition probability is governed by

$$P_{\parallel} = \int S^*_{p_f \underset{\sim}{k}_f} \quad S_{p_i \underset{\sim}{k}_i} \quad dx\,dy \int Z^*_{q_f} \frac{\partial Z_{q_i}}{\partial z}\, dz . \tag{2}$$

From the definition of Z_q in order that $P_{\parallel} \neq 0$, we see that $Z_{q_i} \neq Z_{q_f}$. That is to say in GaSe and GaS the absorption arises from an excitation such as transition 1 in

Figure 1. Although the S-functions are orthogonal the first integral in (2) does not go to zero since even in a direct transition $\underset{\sim}{k}_i \neq \underset{\sim}{k}_f$ because of the finite value of the radiation wave vector. Thus the integral is small but non-zero. When $\underset{\sim}{A}$ is perpendicular to z and lies say along x the transition probability is governed by

$$P_{\perp} = \int Z^*_{q_f} Z_{q_i} \, dz \int S^*_{p_f \underset{\sim}{k}_f} \frac{\partial S_{p_i \underset{\sim}{k}_i}}{\partial x} \, dx \, dy \, . \tag{3}$$

From the definition of $S_{p\underset{\sim}{k}}$ and Z_q it follows that the term involving the gradient is larger in (2) than in (3). Further the orthogonality of the Z_q is likely to be better than that of the S-functions. Thus $P_{\parallel} > P_{\perp}$ in accord with experiment.

Reference

[1]) Z. S. Basinski, D. B. Dove, and E. Mooser, Helv. Phys. Acta *34*, 374 (1961).

Erratum

Helv. Phys. Acta *37*, 389 (1964) L. B. Redei, equations (40) reads:

$$\Omega_+ \, m_0 = 0 \, ,$$

$$\Omega_+ \, h(\boldsymbol{k}) = -\int \frac{g \, \varrho(k)}{\phi^-(w)} \, h(\boldsymbol{k}) \, d\boldsymbol{k} \oplus \left[h(\boldsymbol{k}) + g \, \varrho(k) \lim_{\varepsilon \to 0} \int d\boldsymbol{q} \, \frac{g \, \varrho(q) \, h(\boldsymbol{q})}{(w(q) - w(k) - i \, \varepsilon) \, \phi^-(w(k))} \right]$$