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BAND GAP VARIATION OF GALLIUM SELENIDE UNDER HIGH PRESSURE

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Résumé - Afin de rendre compte de la variation sous pression de la bande interdite de GaSe, nous proposons un modèle dans lequel la nature lamellaire de ce composé est explicitement utilisée. Ce modèle complété par les résultats de calcul de structure de bandes est en très bon accord avec les résultats expérimentaux.

Abstract - Taking into account the lamellar structure of GaSe, we reproduce its complex band gap variation under pressure. The model joint with recent band structure calculation fits very well with experimental data.

Ga Se is layered III-VI semiconductor. The variation of its absorption coefficient under pressure is complex : Although the indirect absorption edge monotonically decreases with pressure, the direct gap first decreases up to 1.3 GPa and then increases at higher pressure. We can account for these variations with a simple model in which we assume that :

- i) the interlayer and interlayer regions are completely independant.
- ii) the deformation potentials depend only upon the nature of the electronic levels.

In order to compare this model with experimental data, we have determined the variation under pressure of the intra- and interlayer distances.

COMPRESSIBILITY

The disconnection of the intra and interlayer regions is the key to our description of the evolution of the cristallographic parameter c under pressure. We write :

$$dc = dc_i + dc_p$$

$$\text{and : } \chi_c = \frac{1}{c} \chi_i + \frac{p}{c} \chi_p$$

$$\text{with } \chi_i^{-1} = B_i = \sum_n B_{oi}^{(n)} p^n = -c_i \frac{dp}{dc_i}$$

$$\chi_p^{-1} = B_p = \sum_n B_{op}^{(n)} p^n = -c_p \frac{dp}{dc_p}$$

where

c : cristallographic parameter

c_p : thickness of one layer of compressibility χ_p in the c direction

$c_i = c - c_p$ interlayer distance in the c direction (compressibility χ_i)

Experimental data were obtained by using a microphotographic method in the diamond anvil cell (D.A.C.). Figure 1 shows the fit between experimental data and this

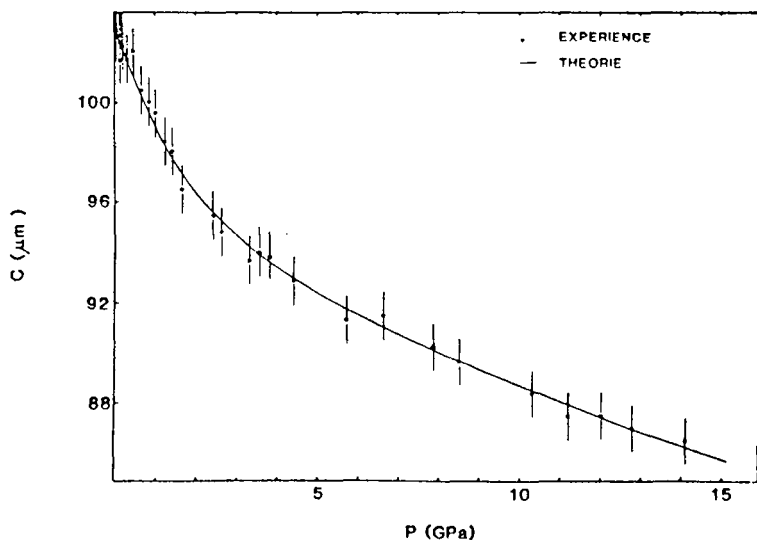


Fig. 1 Length variation of Ga Se under pressure (crystallographic parameter c)

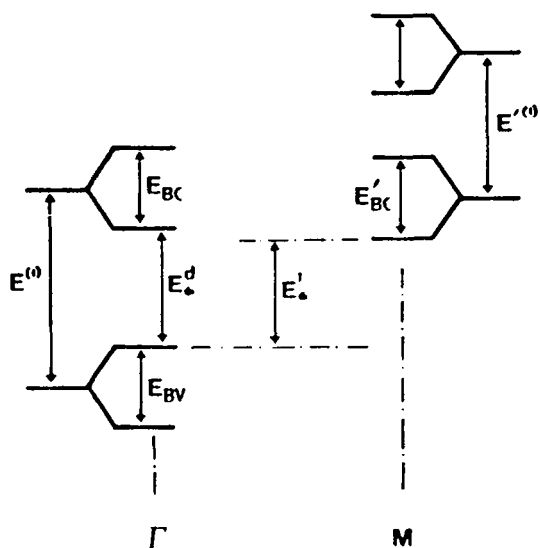


Fig. 2 Schematic band structure of Ga Se.

- E^1 splitting of the s-p gallium levels at the Γ point.
- $E'^{(1)}$ splitting of the P_{xy} gallium levels at the M point.
- E_{BV} , E_{BC} splitting of the P_z selenium levels in the valence and conduction bands.
- E'_{BC} splitting of the P_z gallium levels in the conduction band.

model. We have found $(6,0 \pm 0,2)10^{-3} \text{ GPa}^{-1}$ and $(59,2 \pm 2) 10^{-3} \text{ GPa}^{-1}$ for the intra and intercompressibilities. The ratio $\chi_i(0)/\chi_p(0) \approx 10$ is in good agreement with previous Raman results (1). It is not necessary to invoke a phase transition to explain the strong initial decrease of the c parameter.

ABSORPTION COEFFICIENT

The atmospheric pressure band structure is shown in figure (2). The splitting $E^{(1)}$ at the Γ point ($E'^{(1)}$ at the M point) of the s.p. gallium levels (p_{xy} at M) is due to the intralayer interaction. Splittings E_{BV} , E_{BC} at Γ (E'_{BC} at the M point) of the P_z selenium levels (P_z gallium levels at M) are due to the inter-layer interaction. Electronic levels (s-p, p_{xy}) localised in a layer are assumed to depend only on the intralayer distance ; The P_z levels pointing in the inter-layer region depend only on the interlayer distance. So with the notations of figure 2 :

$$\frac{dE_G^d}{dP} = \frac{dE^{(1)}}{dc_p} \frac{dc_p}{dP} - \frac{1}{2} \frac{dE_{BC}}{dc_i} + \frac{dE_{BC}}{dc_i} \frac{dc_i}{dP}$$

for the direct gap and :

$$\frac{dE_G^i}{dp} = -\frac{1}{2} \frac{dE'^{(1)}}{dc_p} - \frac{dE^{(1)}}{dc_p} \frac{dc_p}{dP} - \frac{1}{2} \frac{dE_{BV}}{dc_i} + \frac{dE'_{BC}}{dc_i} \frac{dc_i}{dP}$$

for the indirect one.

All linear deformation potentials $\frac{dE^{(1)}}{dc_p}$, $\frac{dE'^{(1)}}{dc_p}$, $\frac{dE_{BV}}{dc_i}$, $\frac{dE_{BC}}{dc_i}$ and $\frac{dE'_{BC}}{dc_i}$ are

assumed to be constant and negative.

In order to compare this model with experimental results, we have performed transmission measurements in a D.A.C. with the electrical field perpendicular to the c axis of the sample.

The direct gap was obtained after subtraction of the indirect absorption by using the Elliot-Toyozawa model (3).

Figures 3 and 4 show the fit of the model to experimental data. The pressure coefficients for the two gaps are :

$$\frac{dE_G^d}{dP} \Big|_{P=0} = - (3,4 \pm 1) \times 10^{-2} \text{ et } \text{GPa}^{-1}$$

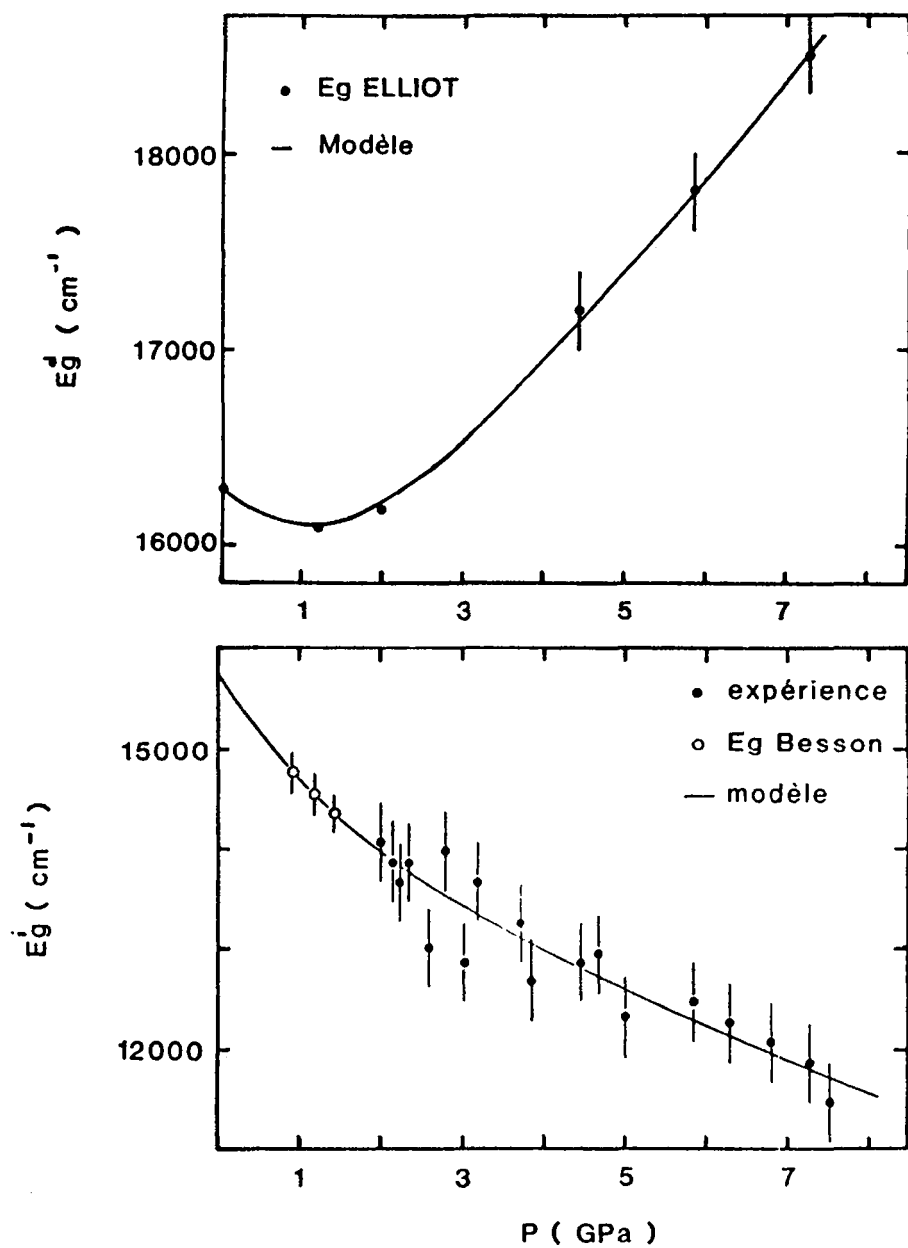


Fig. 3 and 4
Variation of the direct gap (upper figure) and indirect gap (lower figure) of Ga Se under pressure.

$$\frac{dE_G^i}{dP} \quad P=0 = - (14 \pm 1) \times 10^{-2} \text{ eV GPa}^{-1}$$

$$\text{with } \frac{dE^{(1)}}{dc_p} \sim - (2,41 \pm 0,02) \text{ eV } \text{\AA}^{-1} \text{ (s-p gallium levels)}$$

$$\frac{dE'^{(1)}}{dc_p} \sim - (5,1 \pm 0,1) \text{ eV } \text{\AA}^{-1} \text{ (p}_{xy} \text{ gallium levels)}$$

$$\frac{dE_{BV}}{dc_i} \sim \frac{dE_{Bc}}{dc_i} \sim \frac{dE'_{Bc}}{dc_i} \sim - (0,53 \pm 0,01) \text{ eV } \text{\AA}^{-1} \text{ (p}_z \text{ levels)}$$

All these results are consistent and the pressure coefficients for the two gaps are in good agreement with previously published values (4).

In conclusion, we can note that the behaviour of electronic levels under pressure in Ga Se may be quantitatively explained by its lamellar properties. The initial decrease of the direct gap is due, according to this model, to the high compressibility at $P = 0$ of the interlayer region, and the strong decrease of the interlayer compressibility leads to an increase of the direct gap for high pressure.

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