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A. Polian, K. Kunc, J. Rossat-Mignod. INELASTIC NEUTRON SCATTERING AND LATTICE DYNAMICS OF THE LAYER SEMICONDUCTOR GaS. Journal de Physique Colloques, 1981, 42 (C6), pp.C6-295-C6-297. 10.1051/jphyscol:1981685 . jpa-00221621

HAL Id: jpa-00221621

<https://hal.science/jpa-00221621>

Submitted on 4 Feb 2008

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INELASTIC NEUTRON SCATTERING AND LATTICE DYNAMICS OF THE LAYER SEMICONDUCTOR GaS

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Abstract.- Measurements of the phonon dispersion curves of GaS in the $\Gamma \rightarrow M$ and $\Gamma \rightarrow K \rightarrow M$ directions by inelastic neutron scattering have been performed. They show a non dispersive behaviour of the LA phonons in both directions. A Rigid Ion Model (RIM) with anisotropic effective charges and Axially Symmetric Forces (ASF) is constructed from these data and discussed.

1. Experiment.- Inelastic neutron scattering experiments were performed on the layer crystal GaS on the IN3 and IN8 spectrometers at the ILL and DN1 at the C.E.N.G. Two experimental configurations were used allowing to obtain the phonon dispersion in the $\Gamma \rightarrow M$ and in the $\Gamma \rightarrow K \rightarrow M$ directions respectively. The experimental results shown in figure 1 match the earlier measurements^(1,2) and confirm the fact that, in the $\Gamma \rightarrow M$ direction, the LA mode is non-dispersive from $\vec{k}_v(0.25,0,0)$ to the zone boundary. Similar features are found in the $\Gamma \rightarrow K$ direction and there is no dispersion between M and K. The B_2 TA mode shows a similar behaviour.

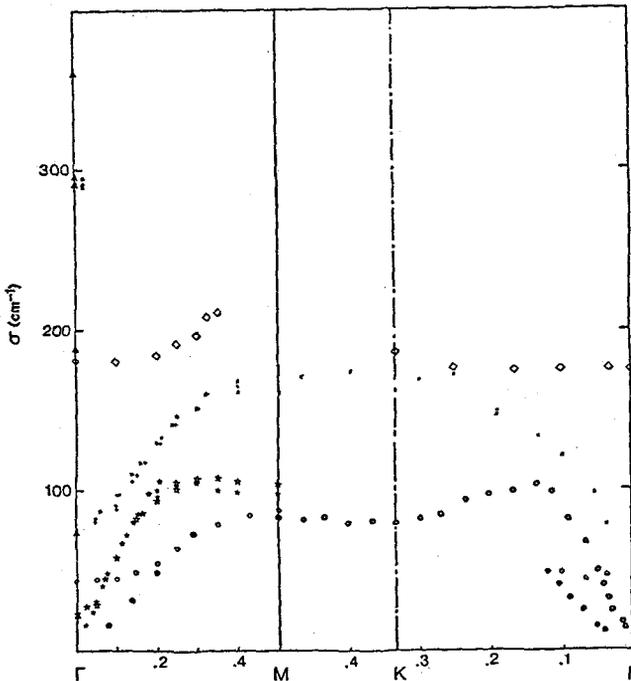


Fig. 1 : Experimental dispersion curves in the layer plane. Each symbol corresponds to a phonon with a different symmetry. The phonons vibrating parallel to the y-axis are not shown here.

The layered nature of the crystal is reflected in the quadratic dispersion at small wave vector of the out-of-the-layer-plane TA mode $\nu = \alpha\zeta + \beta\zeta^2$: with frequency in Hz and reduced wave vector $\zeta = |\vec{k}|/|\vec{k}_M|$, $k_M = 4\pi/a\sqrt{3}$, our measurements yielded $\alpha = 5 \times 10^{-12} \text{ s}^{-1}$ and $\beta \approx 10.5 \times 10^{-12} \text{ s}^{-1}$. As β/α is zero in usual three-dimensional crystals, and 10 in graphite, the present value of $\beta/\alpha = 2$ indicates the degree of bidimensionality.

2. Lattice Dynamics.- We used a Rigid Ion Model (RIM) associated with Axially Symmetric Forces (ASF). The RIM is applied with an anisotropic effective charge tensor :

$$Z^* = \begin{pmatrix} Z_1 & 0 & 0 \\ 0 & Z_1 & 0 \\ 0 & 0 & Z_2 \end{pmatrix}$$

in order to reproduce the anisotropy of the LO - TO splits at the zone center.

The set of 5 central forces (10 parameters A_i, B_i ; $i = 1,5$) represents : interaction n° 1 : Ga - Ga first neighbours; n° 2 : Ga - S first neighbours; n° 3 : S - S interlayer; n° 4 : Ga - Ga second neighbours (intralayer,intercell); n° 5 : Ga - S second neighbours.

3. Discussion.- The ASF parameters A_3 and B_3 are calculated from the rigid layer modes E_{2g} (23 cm^{-1}) and B_{2g} (43 cm^{-1}), the other ones are obtained by least square fit to neutron data. The effective charges are obtained from LO - TO splits of the E_{1u} modes ($Z_1 = 0.9 |e|$) and A_{2u} modes ($Z_2 = 0.44 |e|$).

The dispersion curves calculated in the $\Gamma \rightarrow M$ direction are compared in figure 2. In spite of its simplicity, the model accounts well for all the zone center modes and provides elastic constants in good agreement with values obtained by Brillouin scattering⁽³⁾. On the contrary, the non-dispersive behaviour of the LA phonons in the $\Gamma \rightarrow M$ direction could not be reproduced. While a flat region in the

dispersion of TA modes was already observed in other materials like Si or Ge, a similar behaviour for the LA does not appear in other semiconducting materials.

A tentative explanation of this dispersion could be a coupling between the A_1 (LA)

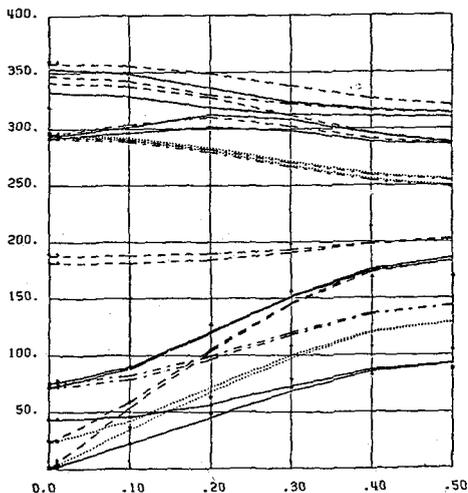


Fig. 2 : Theoretical dispersion curves in the $\Gamma \rightarrow M$ direction.
 — : B_1 modes; ... : B_2 modes
 --- : A_1 modes; -·- : A_2 modes.

mode and the B_1 (E_{1g} in Γ) mode.

Owing to the use of anisotropic effective charge, the present model is able to describe the angular dispersion of the zone center polar phonons. Due to the high symmetry of GaS, the only experimental data available are those parallel and perpendicular to the c-axis so that the prediction cannot be checked. We preferred thus to show in figure 3 the dispersion predicted by the same model rather for γ -GaSe ($Z_1 = 0.84 |e|$; $Z_2 = 0.39 |e|$) a closely related structure in which, however the different stacking and consequently lowered symmetry made possible to obtain more complete data^(4,5).

Large polarisability of bonds in GaS, which is suggested by the space distribution of electronic charges⁽⁶⁾ and shown by the high intensity of the Raman allowed lines raises some doubts about the adequacy of RIM for the description of the lattice dynamics of GaS. It is very likely that any of the standard dipole models (shell, d.d.m. etc.) would be

more satisfactory. It is questionable, however, whether the introduction of polarizable ions *alone*, would be sufficient to explain the non-dispersive behaviour of the A_1 (LA) and B_2 (TA) branches : looking for a description accounting explicitly for the large bond-charges showing up between the Ga atoms would probably be more appropriate.

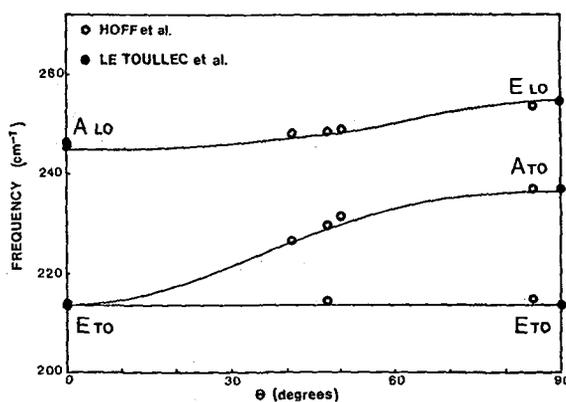


Fig. 3 : Angular dispersion of the polar modes of GaSe.

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