Optical Phonons and Polaritons in $CdAs_2$

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Abstract – Oscillation frequencies of crystalline lattice $CdAs_2$ are calculated in Keating's model. The comparison of the long-wave frequencies and experimental data is lead. The effects of numerical calculation of phonon spectrums are presented in the most symmetrical points and directions of a Brillouin zone, and density of states $CdAs_2$ are also presented. Besides, theoretical examination of an infrared variance of light and a spectrum of polaritons is carried out.

Crystals $CdAs_2$ concern to a major group of semiconductor linking type $A^{II}B^{V}_2$ which possess a series of interesting physical properties and are perspective materials for electronic technique and optoelectronics. In particular, $CdAs_2$ is characterized by a high transparence in IR fields of a spectrum, and also by the significant anisotropy of electrical and optical properties. By present time for many linkings of the specified group the technology of reception of monocrystals is fulfilled and both theoretical and experimental examinations of some physical properties are lead. By present time examination of lattices dynamics $CdAs_2$ is presented by experimental works [1, 2], where spectrums of infrared reflection and uptake are gained. Theoretical examination of properties of symmetry of the lattice oscillations is carried out in work [3].

$CdAs_2$ crystallizes in tetragonal singonia with space group D^{10}_4. The Unit cell contains six particles, hence it is necessary to expect 18 lines in a spectrum of a crystal. Each atom Cd is surrounded by four atoms As, and each atom As – two atoms As and two atoms Cd. Such crystalline structure is rather unusual, that distinguishes $CdAs_2$ from other crystals of group $A^{II}B^{V}_2$. According to the group-theoretic analysis which was lead in work [3], normal oscillations with symmetry Γ_2 and Γ_5 are active in infrared uptake, normal oscillations with symmetry Γ_1, Γ_3, Γ_4 and Γ_5 are active in the Raman scattering too. It is necessary to expect occurrence of 6 lines in spectrums of infrared uptake. Two lines appear at polarization of light, which is parallel to tetragonal axis of a crystal, and four lines – at perpendicular polarization.

In the given work the effects of numerical calculation of the lattice oscillations $CdAs_2$ are presented to Keating's models [4]. This model has been used by us for calculations of the full phonon spectrums, distribution functions of vibrational frequencies, dependence of a heat capacity on temperature for crystals ZnP_2 and CdP_2 in works [5, 6]. For diminution of a number of independent parameters in Keating's model we were restricted to interaction of the first and second neighbours. The analysis of cross distances between atoms allows to take into account two constants of the central interaction between Cd–As and As–As. Off-center interaction was considered by four angular stationary values. Coulomb forces were considered in model of the rigid ions and calculated on Evald's method. The parameters of power interaction given in Table 1 were defined from comparison of the observational and theoretical long-wave frequencies, active in IR fields [2]. Thus Hooke-Jeeves's method of minimization was used with restrictions [7]. The structural data used in calculation, was taken from work [2].

Table 1. Parameters of power interaction

Parameters, $\times 10^3$ dyn/sm	$CdAs_2$
α_1	35.1
α_2	79.3
β_1	6.0
β_2	5.4
β_3	3.0
β_4	12.0
q (a charge in a.e.)	0.7

The long-wave phonon frequencies of crystal $CdAs_2$ calculated and observationally measured by us are given in Table 2.

Table 2. The long-wave frequencies of phonons

Symmetry	Frequencies of phonons ν_{TO}/ν_{LO}, sm^{-1}	
	Experiment [2]	Theory
Γ_1		217
Γ_2	83 / 88 202 / 213	75 / 81 213 / 217
Γ_3		74 142
Γ_4		185 256
Γ_5	51 / 55 120 / 126 202 / 208 245 / 247	59 / 69 116 / 116 198 / 201 246 / 246

In Figure 1 the calculated phonon spectrums in the most symmetrical directions and points of a Brillouin zone, and also density of states $CdAs_2$ are given.

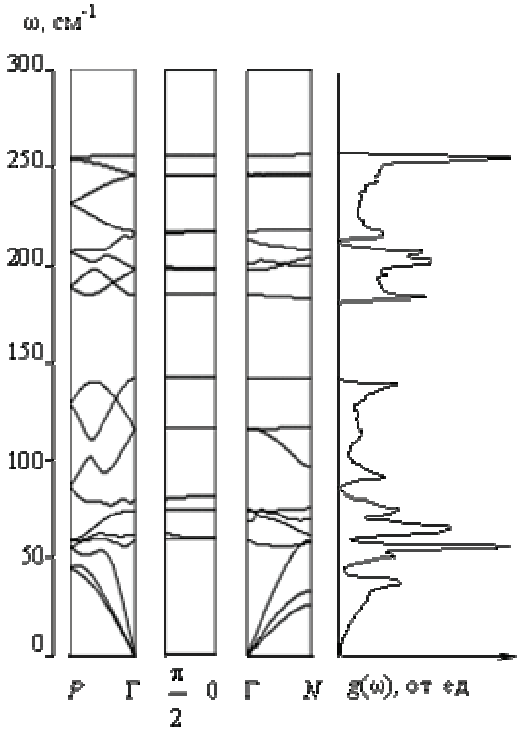

Fig. 1. A phonon spectrum and density of states $CdAs_2$

The model developed by us has allowed to carry out theoretical examination of an infrared variance of light and a spectrum of polaritons in semiconductor crystals $A^2B_2^5$. The dependence of coefficient IR of reflection of light on frequency and an angle between a wave vector and a direction of an optical axis in crystal $CdAs_2$ is given in Fig. 2.

From Figure 2 we can see, that frequencies with symmetry Γ_3 and Γ_4 can simultaneously be shown at the intermediate orientations of a wave vector in a spectrum of reflection. The good consent of a theoretical and experimental curve of a reflectivity in crystal $CdAs_2$ is reached for $\theta = \frac{\pi}{2}$, however for $\theta = 0$ there is a small discrepancy with experiment in the field of frequencies of ~100 cm^{-1}.

The calculated phonon spectrum at the centre of a Brillouin zone allows to explore a spectrum of polaritons, which is useful at making optical quantum generators and the amplifiers using effect of the forced Raman effect of light on polaritons. In Figure 3 the qualitative spectrum of polaritons spreading perpendicularly (a direction (q,0,0)) and in parallel (a direction (0,0,q)) to a tetragonal axis in crystal $CdAs_2$ is figured.

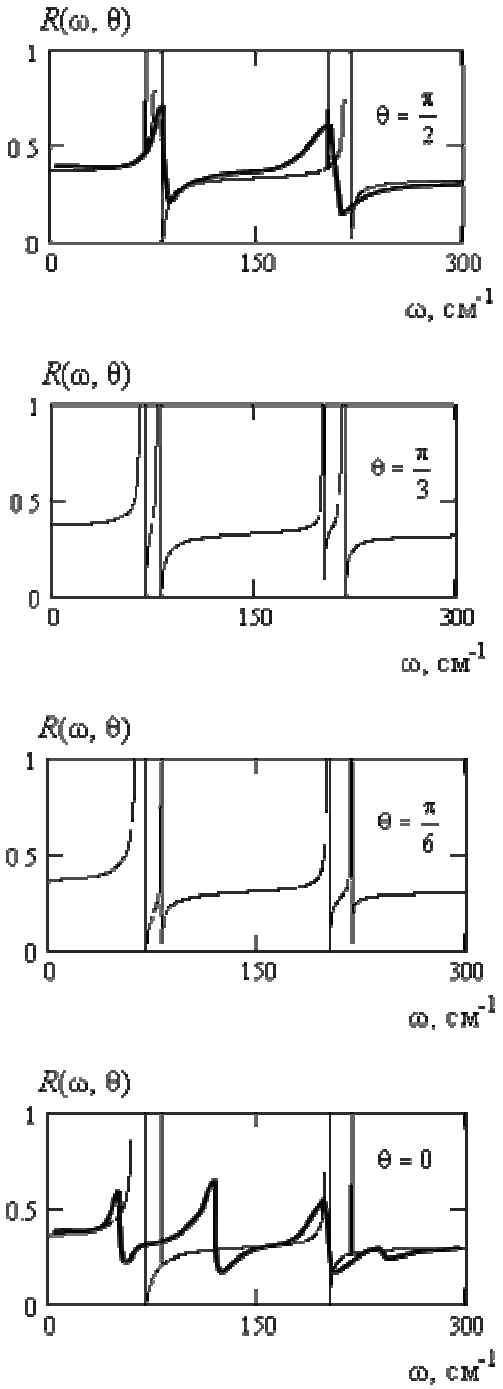

Fig. 2. Dependence of coefficient IR of reflection on frequency and an angle between a wave vector and a direction of a tetragonal axis in crystal $CdAs_2$. A thin line shows calculation, a fat one – experiment [2]

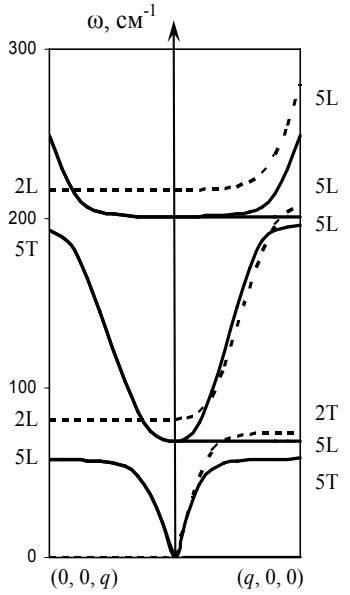

Fig. 3. A spectrum of polaritons $CdAs_2$

The frequencies of ordinary (E⊥*z*) polaritons are shown by a continuous line, unusual (E∥*z*) – by dotted line. Presence of forbidden regions in a spectrum of polaritons means that the light with corresponding frequency and polarization should be completely reflected from a crystal.

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