

Phonon dispersion in aluminium arsenide and antimonide

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Abstract. The phonon dispersion curves for aluminium arsenide and antimonide have been investigated by using a deformation bond approximation model. The results obtained from this model are compared with the experimental values wherever it is available. Since there is no complete experimental phonon dispersion curves for AIAs, we could not compare our calculated results, but the results of AlSb have been compared with the inelastic neutron scattering measurements at 15 K. However, we compare the phonon frequencies of AIAs and AlSb at critical points of the Brillouin zone obtained by our calculations and Raman spectroscopy measurements. This model predicts the phonon modes satisfactorily in all the symmetry directions of the Brillouin zone (BZ). The spectrum has similar features as observed in other III–V compound semiconductors.

Keywords. Semiconductor; phonons; lattice dynamics; neutron scattering.

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1. Introduction

The lattice dynamical properties of tetrahedrally bonded Al-containing III–V compounds are interesting, since understanding its phonon properties is crucial for technological application. These include heterojunction bipolar transistor, Bragg reflector superlattices, solid state lasers and high electron mobility transistors. Information on phonon dispersion is important in considering the electronic conduction, the non-radiative relaxation process of electrons and so on. However, not much studies have been conducted to understand the role played by phonons in these compounds although the AIAs and AlSb are the partners of the vastly used and studied superlattices containing GaAs/AIAs and GaSb/AlSb which are of great interest [1–7]. In all the Al-containing III–V compounds, the experimental data is only available for AlSb at 15 K alone [8]. Recently Strauch *et al* [8] have determined the phonon dispersion curves in symmetry directions for AlSb by using inelastic neutron scattering at 15 K. They have also performed the model calculation by using bond charge model, where the model parameters have been obtained from a least square fit. In a recent paper, Molinas-Mata *et al* [9] have studied the phonon dispersion curves along [110] and [111] direction of BZ and internal stresses in some III–V compounds including AIAs and AlSb by using the planer bond charge model (PBCM). In this calculation, the PBCM has been fitted to the [100] and [111] inelastic neutron scattering data. Also, in the

case of AIAs, the mass approximation method has been adopted to calculate the phonon dispersion curves (PDC) by considering GaAs as the reference material. With respect to AIAs, one of the typical III–V compound semiconductors, no measurement on phonon dispersion has been performed so far, because it is difficult to grow sufficiently large single crystals of good quality which are free from oxidation. In the early stage of studying the phonon structure in AIAs, several workers have reported phonon frequencies at critical points in Brillouin zone (BZ) by various experimental methods [10, 11, 15, 16]. The phonon dispersion of AIAs along the Δ [12–14] and Λ directions have also been obtained using confined optical phonons in GaAs/AIAs superlattices. In recent studies, Spencer *et al* [17] and Wagner *et al* [18] have measured second order Raman bands in AIAs layers on GaAs and reported the overtone frequencies at the X and L -points. Quite recently, Azuhata *et al* [19] have measured the second order Raman spectra in AIAs layer grown on a GaAs substrate by Raman spectroscopy. They have also calculated the phonon dispersion curves by using the modified version of adiabatic bond charge model but the values of parameters have been obtained from *ab initio* calculations for AlSb by using a similar approach. Thus a realistic lattice dynamical model still seems to be useful for the theoretical studies of phonon properties for Al-containing III–V compound semiconductor to understand the phonons in them.

In the present paper, we report the results of the phonon dispersion curves for AIAs and AlSb by using the formalism of a simplified version of the deformation dipole model [22], called deformation bond approximation (DBA) model [23]. In §2 the model is described briefly, and the results and discussion in §3.

2. Model

The deformation dipole model is based on the hypothesis that an overall charge rearrangement due to overlap that produces a net concentration of positive charges at the bonds. During lattice vibration, a new charge distribution is set which, in principle, may be described in terms of a multiple expansion. Kunc *et al* [22] incorporated this idea by considering the terms up to dipole which are assumed to be on the ion site. Fifteen parameters take into account the polarization and deformation of electronic orbitals. These fifteen parameters are very difficult to find due to very limited number of input parameters, which is difficult to employ for the study of lattice vibrations. Kunc *et al* [23] have simplified this model for practical purposes and used for several compound semiconductors. This simplified version of deformation dipole model is known as deformation bond approximation and is quite successful in explaining the phonon properties [24]. The simplification consists: (i) In assumption, reducing the number of independent deformabilities. (ii) In the neglect of “nonlocal electronic polarizabilities”. By neglecting the nonlocal polarizabilities, we get a model equivalent to that of Karo and Hardy [25, 26]. This approximation is formally equivalent to the shell model in the case of ionic and semi-ionic crystals [22].

The dynamical matrix corresponding to deformation bond approximation (DBA) model is written as [23]

$$C(q) = C^{sr}(q) - M^{-1/2}(e + N^+)(I - Ba)(e + N)M^{-1/2}, \quad (1)$$

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Table 1. Input and output parameters for AlSb and AlAs. The value of a , ω , C_{11} , e_{14} and α are in Å, THz, dyne/cm², esu/cm and cm⁻⁹ respectively and are taken from refs [19, 31–34]. The output parameters are in units of 10⁵ dyne/cm.

	Input parameters		Output parameters		
	AlSb	AlAs	AlSb	AlAs	
a	6.1300	5.6600	A	-0.3816	-0.4489
ω_{TO}	9.5700	10.8100	B	-0.3150	-0.3212
ω_{LO}	10.2100	12.1300	C_1	-0.0072	-0.0081
ϵ_∞	15.6800		D_1	-0.0061	-0.0067
C_{11}	0.894	—	F_1	0.0010	0.0013
C_{12}	0.443	—	C_2	0.0037	0.0039
C_{44}	0.416	—	D_2	0.0048	0.0055
e_{14}	-2.04	—	F_2	-0.0056	0.0059
α_1	0.221	—	γ_1	0.5711	0.6401
α_2	10.221	—	γ_2	0.0011	0.0017

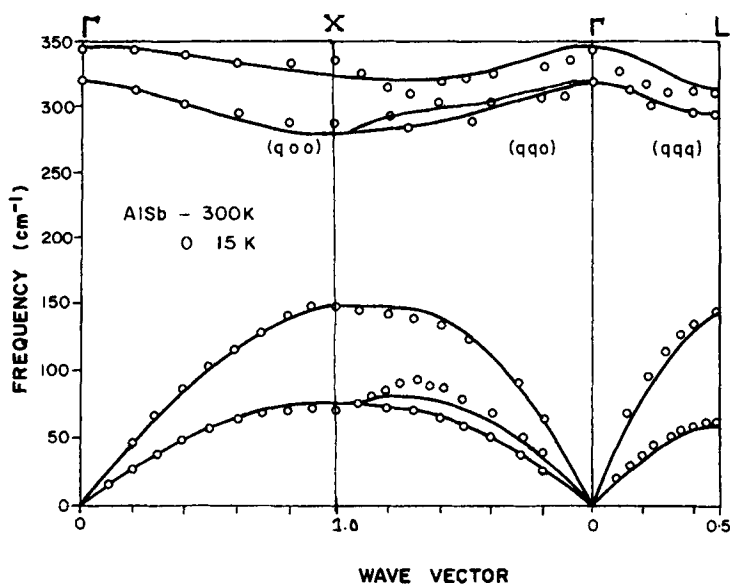


Figure 1. Phonon dispersion curves of AlSb. Experimental points are taken from [8, 21].

where I is a unit matrix, $C^{sr}(q)$ is short range matrix, and the matrices N and a are the Fourier transform of the deformability and polarizability respectively [23, 27]. The matrix B in the dynamical matrix is the contribution from the Coulomb coefficients and can be found in [28, 29]. We have also calculated the PDC for II–VI compound semiconductors by using the same theoretical approach [30]. The results are in good agreement with experiment. The present model has ten parameters and most of them are determined from their relations with some macroscopic experimental data. These are listed in table 1, where A, B, C_i, D_i, F_i ($i = 1, 2$) are the short range force constants, and are given in ref. [23]. The input parameters are taken from [31, 32] and presented in table 1 along with

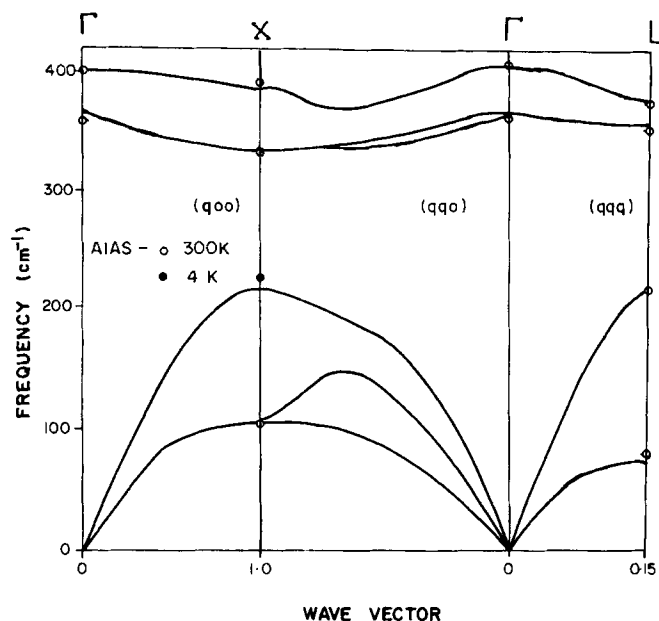


Figure 2. Phonon dispersion curves of AlAs. Experimental points are taken from [19, 34].

output parameters. The notations have their usual meaning. The values of the force constants listed in table 1 are quite reasonable and have not attained any unphysical value though they are partially fitted to macroscopic properties.

3. Results and discussion

The calculated phonon dispersion curves of AlSb by using the model mentioned above are shown in figure 1. The calculated results are compared with the measured data at 15 K [8] due to the non-availability of room temperature experimental data for all the wave vectors in the symmetry directions of Brillouin zone (except at Γ -point). This can also be justified from the fact that the Γ point frequencies are nearly the same at 300 K and 15 K [8]. It is revealed from figure 1 that the calculated results using DBA model agree reasonably well with the available neutron scattering data.

The dispersion of both optical and acoustic phonons are explained more or less satisfactorily in the Δ direction for AlSb. However, minor disagreement for LO and TA modes along X-direction can be observed. Also, the LO and TO branches are almost parallel from Γ to X point. The phonon modes in Σ -direction of the Brillouin zone are also reproduced reasonably well from the present model. The other important feature of the PDC, the flattening of the acoustic branches which is observed in almost all the III-V compound semiconductors has been correctly predicted from the present model calculations.

The calculated phonon dispersion curves for AlAs by using the modified version of deformation dipole model are presented in figure 2. For the calculations of PDC of AlSb except the mass and lattice parameters very limited informations about the microscopic

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Table 2. Phonon frequencies at critical points of the symmetry direction of the Brillouin zone for AlAs.

Mode	Experiment	Phonon frequency (cm ⁻¹)		
		Previous work		Present work
		<i>Ab initio</i> calculation ^e	BCM ^f	DBA
LO(Γ)	404 ^{a,g} , 404 ^{b,g} , 402 ^{f,g}	403	399	400
TO(Γ)	361 ^{a,g} , 363 ^{b,g} , 360 ^{f,g}	365	363	365
LO(X)	400 ^a , 396 ^b , 403 ^c , 391 ^f	396	390	385
TO(X)	340 ^a , 338 ^b , 335 ^c , 332 ^f	338	329	335
LA(X)	222 ^c	219	215	213
TA(X)	103 ^a , 103 ^b , 109 ^c , 104 ^f	97	107	104
LO(L)	373 ^d	375	371	375
TO(L)	350 ^a , 350 ^b , 349 ^f	354	348	352
LA(L)	–	214	211	212
TA(L)	83 ^b , 77 ^f	74	78	75

^a[17], $T = 36$ K; ^b[18], $T = 77$ K; ^c[36] $T = 4$ K; ^d[18] $T = 300$ K; ^e[20]; ^f[19], $T = 300$ K; ^gfrom the first order Raman spectra.

Table 3. Phonon frequencies at critical points of the symmetry direction of the Brillouin zone for AlSb.

Mode	Experiment	Phonon frequency (cm ⁻¹)		
		Previous work		Present work
		<i>Ab initio</i> calculation ^c	BCM ^f	DBA
LO(Γ)	337 ^{a,e} , 352 ^b , 337 ^{d,e}	334	337	337
TO(Γ)	317 ^{a,e} , 318 ^b , 317 ^{d,e}	316	318	317
LO(X)	338 ^a , 341 ^b	342	335	331
TO(X)	294 ^a , 294 ^b , 290 ^d	289	292	288
LA(X)	154 ^b	152	153	153
TA(X)	65 ^a , 69 ^b , 70 ^d	64	74	74
LO(L)	320 ^b	325	317	323
TO(L)	306 ^a , 307 ^b , 309 ^d	306	309	307
LA(L)	142 ^a , 147 ^b	148	150	144
TA(L)	58 ^a , 56 ^b , 53 ^d	49	55	53

^a[36], $T = 300$ K; ^b[8], $T = 15$ K; ^c[20] $T = 4$ K; ^d[18] $T = 300$ K; ^efrom the first order Raman spectra; ^f[19], $T = 300$ K.

properties for AlAs are available so far. The phonon dispersion curves for AlAs could also not be compared with the experimental measurements. However, the phonon frequencies at the critical points of the symmetry directions of BZ are listed in table 2 with some experimental data obtained from second order Raman spectra and *ab initio* calculations of Giannozzi *et al* [20]. Thus there is a good agreement between the present calculations and previous experimentally and theoretically obtained values. It can also be seen from figure 2 that all the common features of III–V compound semiconductors have been correctly predicted from the present version of deformation dipole model.

We also present a comparative study of the phonon frequencies for AlAs and AlSb at critical points of the symmetry direction of BZ, calculated by the present model theory and some earlier calculated results in tables 2 and 3 to judge the validity of the present model. It is quite successful in explaining the phonon frequencies at critical points.

Thus we have presented here the results on phonon dispersion curves of AlAs and AlSb using DBA model. The present model has been quite successful in explaining the gross features of PDC of this compound as in the case of other III–V compound semiconductor. We emphasize for the neutron scattering measurements of these compound.

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