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Lattice dynamical properties of MnTe, HgTe and their mixed semiconductor $Mn_xHg_{1-x}Te$

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Abstract. **In the present paper, the phonon dispersion relations, phonon density of states and Debye characteristics of mixed semiconductor $Mn_xHg_{1-x}Te$ and the end members MnTe and HgTe using three-body shell model were studied. The model involves 11 disposable parameters and incorporates the effect of the short-range repulsive interactions up to and including the second nearest neighbours, in addition to the long-range Coulombic interactions in the framework of the rigid-shell model with both the ions polarizable. The comparisons of the theoretical results with the available experimental results were in good agreement.**

Keywords. **Chalcogenides; semiconductor; phonons; thermodynamic properties.**

1. Introduction

There is considerable interest in the study of properties of zinc-blende (ZB) MnTe compound. ZB MnTe is a well-known magnetic semiconductor, which has been an object of intensive studies for the last two decades. Its lattice parameter value is not far from values of several II–VI-type semiconducting compounds and hence such MnTe is often applied as a constituent of II–VI quantum structures, also these are used in spintronic experiments. However, bulk ZB MnTe crystals do not exist in nature because of the metastable character of this phase.

The solid solution of HgTe and MnTe form ternary mixed crystal $Mn_xHg_{1-x}Te$ which belongs to a group of materials known as semimagnetic semiconductors. These crystals are narrow-gap semiconductors with a variable energy gap, which depends on composition x and which can be either positive or zero. The interest in these materials have been rapidly increased, prompted by the fact that the presence of a magnetic constituent in the semiconductor lattice is expected to lead to new physics effects as a result of exchange interactions. However, the two-mode behaviour of the phonons in the mixed $Mn_xHg_{1-x}Te$ system was studied. The infrared reflection spectra of $Mn_xHg_{1-x}Te$ were measured in the optical region from 50 to 300 cm^{-1} by Gebicki and Nazarewicz.[1] They also applied the random element as a displacement model to calculate numerically the long wavelength optical phonon frequencies in the mixed crystals as a function of composition.

In recent times, Mnasri *et al*[2] have calculated the electronic, lattice dynamical and mechanical properties of compounds CdTe, ZnTe, MnTe, MgTe and HgTe having ZB structure and their ternary alloys $Cd_{1-x}Zn_xTe$, $Cd_{1-x}Mn_xTe$, $Zn_{1-x}Mn_xTe$, $Cd_{1-x}Mg_xTe$ and $Cd_{1-x}Hg_xTe$ using the empirical pseudopotential method (EPM).

In recent times the lattice dynamical properties of HgTe, CdTe, and their ternary alloy $Cd_xHg_{1-x}Te$ in ZB phase using the three-body shell model (TBSM) were studied.[3] In this work this model was used to study the lattice dynamical properties of HgTe, MnTe and their ternary alloy $Mn_xHg_{1-x}Te$.

2. Potential model

The TBSM incorporates the effect of three-body and the short-range repulsive forces up to and including the second nearest neighbours, in addition to the long-range Coulombic interactions in the framework of rigid-shell model (RSM) according to Woods *et al*[4] with both the ions polarizable. The general formulation of TBSM remains in the harmonic approximation can be derived from the work by Cochran and his collaborators[5] who have developed the framework of RSM.

The lattice dynamical calculations are carried out by using a TBSM described in the literature.[6,7] According to Kushwaha,[6] the harmonic potential energy per unit cell for ZB structure compounds can be written as

$$\varphi = \varphi^{SM} + \varphi^{TB}, \quad (1)$$

where φ^{SM} and φ^{TB} are the potential energies of the binary crystal in the framework of RSM and three-body interaction, respectively.

Blackman sampling technique[8] is used to calculate the phonon density of states. In this technique the entire

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frequency range is divided into a number of small intervals of width $\Delta\nu = 0.1$ THz and all the frequencies falling into these intervals are counted with their statistical weights and from these values the graph for the frequency distribution $g(\nu)$ was plotted. For the calculation of phonon density of states and the Debye characteristics temperature the method given in the literature was used.[9]

3. Results and discussion

3.1 *Lattice dynamical properties*

In this model, 11 parameters such as two-body short-range interaction (A, A_1 and A_2), three-body short-range interaction (γ_1, γ_2 and γ_3), electronic polarizability (α_1 and α_2), distortion polarizability (d_1 and d_2) and effective charge parameter (Z') were calculated. The procedure of calculation of force parameters for the compounds MnTe, HgTe and $Mn_xHg_{1-x}Te$ are given elsewhere.[6] The input and the output data for the compounds MnTe, HgTe and $Mn_xHg_{1-x}Te$ are given in table 1.

The force parameters for the end members MnTe and HgTe are taken from table 2 and calculated the values of force parameters for the mixed system $Mn_xHg_{1-x}Te$ at $x = 0.35$ using Vegard's Law.[10] These are also listed in table 2. The value of non-randomness parameter λ is calculated by fitting to one of the experimental long-wavelength optical phonon frequency taken from infrared reflection spectra[1] of $Mn_xHg_{1-x}Te$.

The calculated phonon dispersion relations for MnTe, HgTe and $Mn_xHg_{1-x}Te$ at $x = 0.35$ along three high symmetry directions are given in figures 1–3, respectively, along with their available experimental results[11] for MnTe at the zone centre and for HgTe.[12] As the complete experimental phonon spectra for MnTe system is not available in the

Table 1. Input data taken from references 26 and 29.

	Experimental values		
Quantities	MnTe	HgTe	Units
a	3.22	3.21	Å
C_{11}	5.20	5.40	10^{11} dynes cm^{-2}
C_{12}	3.10	3.80	10^{11} dynes cm^{-2}
m_1	186.58	335.02	10^{-24} g
m_2	211.82	211.82	10^{-24} g
$\nu_{LO}(\Gamma)$	5.08	4.14	THz
$\nu_{TO}(\Gamma)$	4.20	3.54	THz
$\nu_{LO}(X)$	4.44	4.20	THz
$\nu_{TO}(X)$	3.75	2.75	THz
ε_0	9.60	19.13	
ε_∞	7.21	14	
e	4.80	4.80	10^{-10} esu

Table 2. Parameters of the model.

	Value			
Parameters	MnTe	HgTe	$Mn_xHg_{1-x}Te$	Units
A	68.03	55.77	60.06	10^3 dynes cm^{-1}
A_1	6.46	15.99	12.65	10^3 dynes cm^{-1}
A_2	4.41	7.24	3.16	10^3 dynes cm^{-1}
γ_1	1.19	3.07	2.41	10^3 dynes cm^{-1}
γ_2	0.39	1.69	1.24	10^3 dynes cm^{-1}
γ_3	0.13	1.02	0.71	10^3 dynes cm^{-1}
α_1	0.24	0.72	0.55	10^{-24} cm^{-3}
α_2	2.79	12.78	9.28	10^{-24} cm^{-3}
d_1	0.06	0.03	0.04	
d_2	0.75	0.52	0.60	
Z'	0.31	0.51	0.44	

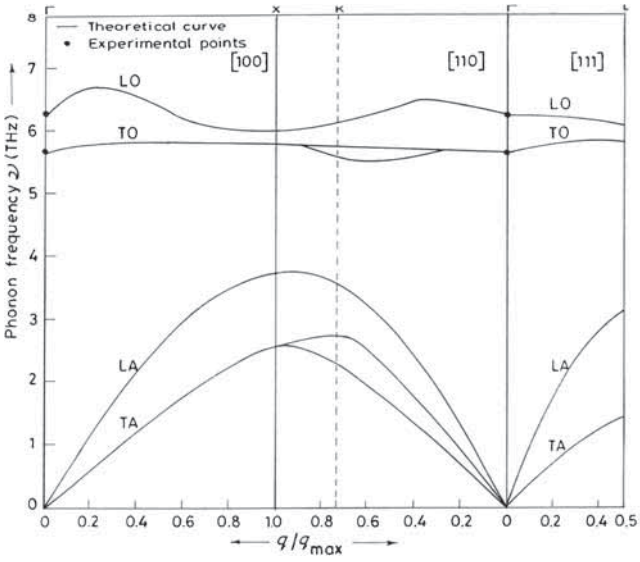

Figure 1. Phonon dispersion relations of MnTe.

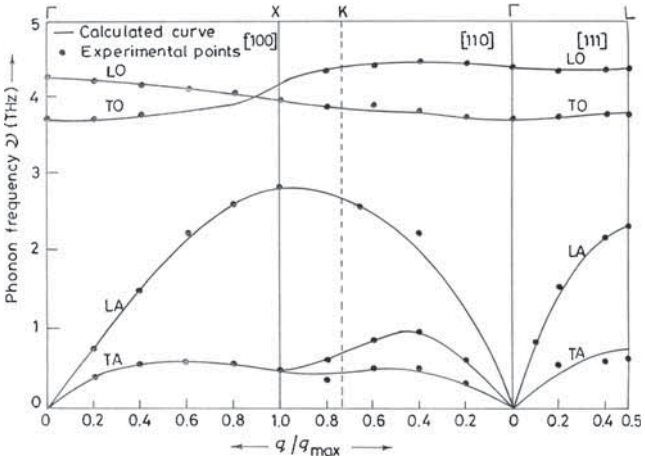

Figure 2. Phonon dispersion relations of HgTe.

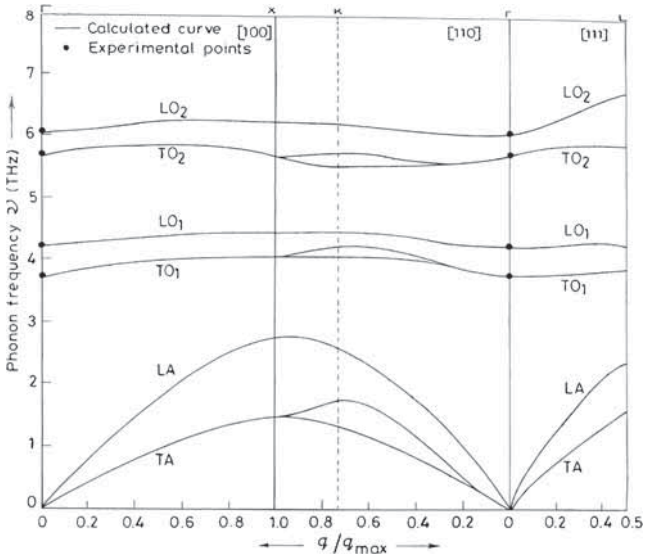

Figure 3. Phonon dispersion relations of $Mn_xHg_{1-x}Te$ at $x = 0.35$.

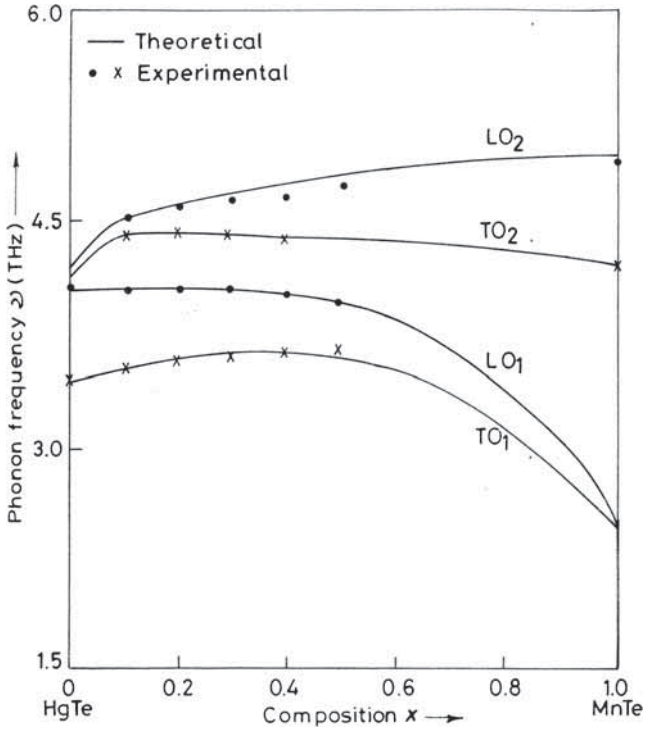

Figure 4. Phonon dispersion in $Mn_xHg_{1-x}Te$ exhibiting two-mode behaviour at zone centre.

literature, it was unable to compare the calculated results at the other points of the Brillouin zone. In the case of HgTe, the transverse acoustic modes show a discrepancy of the order of 5% at L point, while longitudinal acoustic and optic modes are in satisfactory agreement with the experimental results. A good agreement with experimental points at zone centre taken from Gebicki and Nazarewicz[1] for the mixed system.

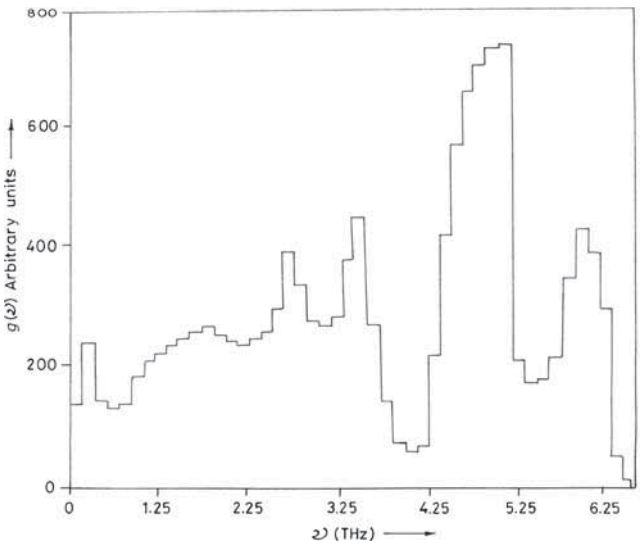

Figure 5. Phonon density of states of MnTe.

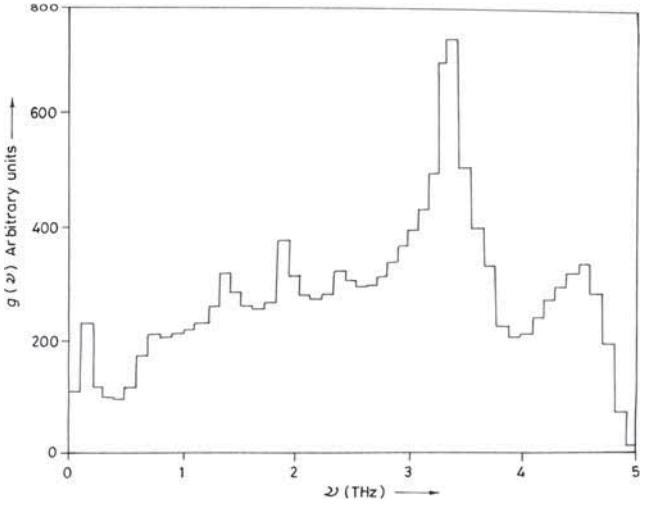

Figure 6. Phonon density of states of HgTe.

Two-mode behaviour of mixed $Mn_xHg_{1-x}Te$ system as a function of composition x at the zone centre is shown in figure 4. Experimental points for the composition range $0 < x < 0.69$ and at $x = 0$ and 1 are also marked from infrared reflection spectra of Gebicki and Nazarewicz.[1] It has been observed from figure 4 that $Mn_xHg_{1-x}Te$ displays two-mode behaviour for whole of the composition range $0 < x < 0.69$ and pure crystal behaviour at $x = 0$ and 1 for HgTe and MnTe, respectively.

The calculated phonon density of states for MnTe, HgTe and $Mn_xHg_{1-x}Te$ are shown in figures 5–7, respectively. The peaks in figure 5 at frequencies 0.125, 2.25, 3.325 and 4.2 THz show transverse acoustic (TA), longitudinal acoustic (LA), transverse optic (TO) and longitudinal optic (LO) modes, respectively. Similarly in figure 6, the peaks at the frequencies 1.75, 2.75, 5.25 and 6.25 THz are due to TA,

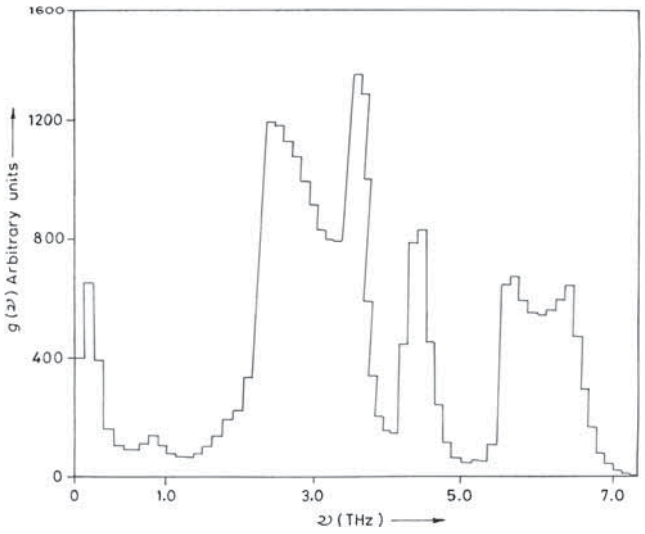

Figure 7. Phonon density of states of $Mn_xHg_{1-x}Te$.

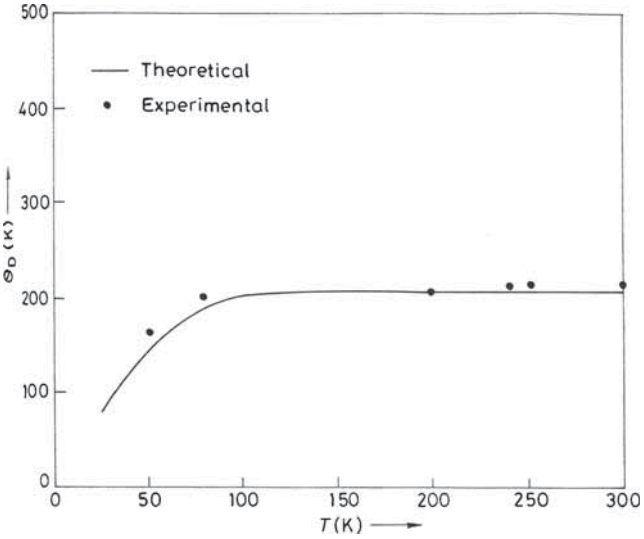

Figure 9. θ_D *vs*. T curve for HgTe.

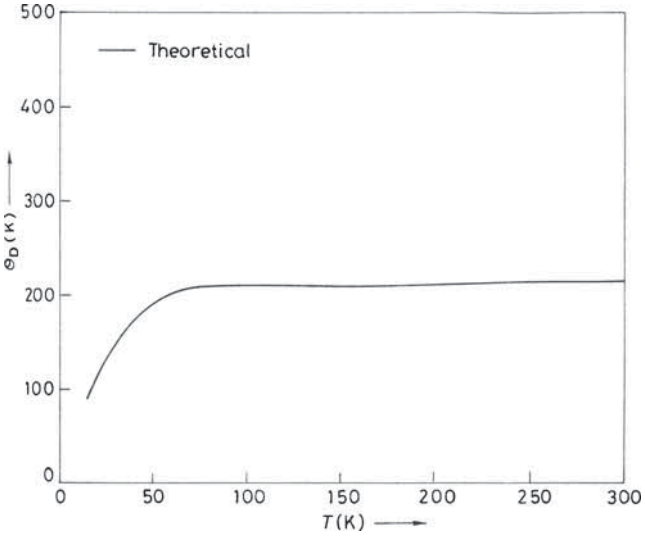

Figure 8. θ_D *vs*. T curve for MnTe.

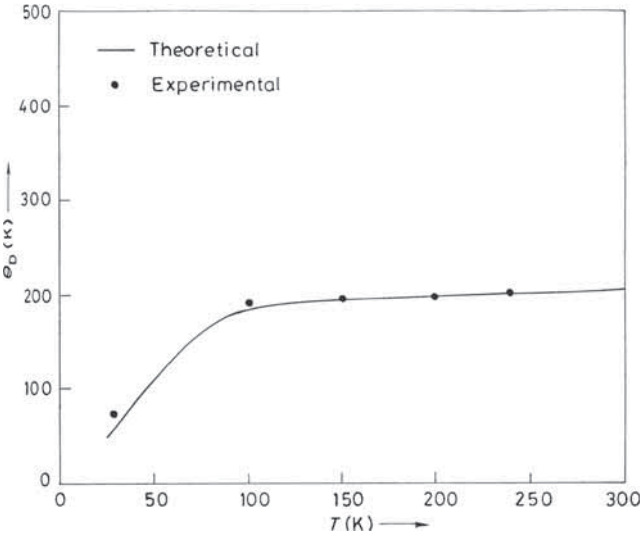

Figure 10. θ_D *vs*. T curve for $Mn_xHg_{1-x}Te$.

LA, TO and LO modes, respectively. Six major peaks in figure 7 at frequencies 0.8, 2.4, 3.6, 4.2, 5.6 and 6.4 THz are due to LA, TA, TO_1, LO_1, TO_2 and LO_2 modes, respectively.

The calculated values of Debye characteristic temperature θ_D are plotted as a function of temperature for MnTe, HgTe and $Mn_xHg_{1-x}Te$ system and are as shown in figures 8–10, respectively. Because of lack of availability of experimental results in MnTe system the results with the experimental values could not be compared. Nagata *et al*[13] have studied the low temperature variation of specific heat with temperature for HgTe and for $Mn_xHg_{1-x}Te$ system at $x = 0.35$ from 10 to 20 K and Vekilov and Rusakov[14] have experimentally studied the specific heat of HgTe from 30 to 150 K. These experimental results are shown in the figures 9 and 10.

4. Conclusions

In the present paper, rigid shell model along with the three-body interactions has been used with both the ions polarizable. Using this model, the phonon dispersion relations, phonon density of states and Debye characteristics temperature for MnTe, HgTe and mixed semiconductor $Mn_xHg_{1-x}Te$ were calculated. Theoretical results are found to be in good agreement with the available experimental results.

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