Lattice vibration spectra of $A_{II(1-x)}B_{II(x)}C_{VI}$ systems

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Abstract. Phonon spectra for mixed systems of II–VI compounds are worked out in an MRI model and the Debye Waller factor evaluated from these phonons are compared with the recent experimental values of Baudour *et al* where some interesting behaviours are reported.

Keywords. Mixed II–VI systems; phonons; two-mode behaviour; Debye Waller factor.

1. Introduction

Recently Baudour *et al* (1989) reported from X-ray measurements the composition dependence of thermal vibrations at room temperature and in some cases at 143 K for some of the II–VI mixed systems. These experimental data are refined for anomalous dispersion and anharmonicity etc when Debye Waller factors (DWF) are deduced. Here, for $Zn_{1-x}Hg_xTe$, DWF varies linearly with x for cation, whereas it is non-monotonic for anion.

In general, such behaviour is not expected and hence a theoretical investigation will be useful in understanding such mixed systems. Since the mixed II–VI systems find important places in technological applications such as solar cells and infrared detectors, such a detailed study is indeed useful.

2. Vibration spectra of $Zn_{1-x}Hg_xTe$

Even though Raman measurements on these mixed systems for zone centre phonons are available, the complete vibration spectra for these mixed systems are sparse. Similarly the calculation of phonons for these mixed systems for the entire Brillouin zone is rare.

Hence, in this paper, a theoretical investigation on the complete vibration spectra and DWF with concentration are presented.

2.1 Model

The most important models for these mixed systems are modified rigid ion model (MRI) and random element isodisplacement model (REI). While the REI model gives only the zone centre phonons the MRI model gives the phonons over the entire Brillouin zone.

Varshney *et al*, as early as 1975, proposed an MRI model for systems like $AB_{1-x}C_x$, where B and C are the anions. Being the only model which could satisfactorily explain the phonons over the whole Brillouin zone and the two-mode behaviour in mixed systems, this has been implemented here for systems like $A_{1-x}B_xC$ where A and B are cations, where such work for II–VI and III–V systems is rarely reported.

Mixed systems of II–VI compounds crystallize in zinc blende structure (Baudour 1989). In the mixed zinc blende lattice of the form $A_{1-x}B_xC$, the cation site consists of fractional amounts of A and B ions proportional to the mixing ratio in the crystal with the anions at their normal site. Short-range and long-range interactions are considered, with short-range, including central and noncentral interactions, up to second neighbours.

The detailed expressions for the evaluation of force constants are derived for the $A_{1-x}B_xC$ -type systems. Noncentral (nearest-neighbour) interactions $\alpha_1, \beta_1, \alpha_2, \beta_2, \alpha_3$ and central (next-neighbours) interactions μ_1, μ_2 and μ_3 are worked out (1, 2, 3 corresponding to AC, BC and AB interactions). Effective charge and lattice constant is assumed to vary linearly following Vegard's law.

In this work, apart from $Zn_{1-x}Hg_xTe$, other systems like $Zn_{1-x}Cd_xTe$ and $Cd_{1-x}Hg_xTe$ are also investigated. Input data and the parameters evaluated are given in tables 1 and 2 for $Zn_{1-x}Hg_xTe$, $Cd_{1-x}Hg_xTe$, $Zn_{1-x}Cd_xTe$.

Table 1. Input data for the evaluation of model parameters: (C_{ij} s are in $10^4 \text{ dyn. cm}^{-2}$; ω s are in cm^{-1}).

System	C_{11}	C_{12}	C_{44}	Ref.	ω_{LO}	ω_{TO}	Ref.	ω_1	Ref.
ZnTe	7.12	4.07	3.13	(a)	207	177	(a)	$\omega_{1,Hg} = 156$ $\omega_{1,Cd} = 153$	(b) (c)
CdTe	5.35	3.68	1.99	(d)	169.5	140.5	(d)	$\omega_{1,Hg} = 131$ $\omega_{1,Zn} = 169$	(c) (c)
HgTe	5.36	3.66	2.11	(f)	138	117		$\omega_{1,Cd} = 148$ $\omega_{1,Zn} = 184$	(e) (b)

$\omega_{1,Hg}$ in ZnTe and $\omega_{1,Zn}$ in HgTe are fixed from the mass defect vs impurity mode graph in ref. (b).

(a) Vegelato *et al* 1974

(b) Gaur *et al* 1971

(c) Barker and Sievers 1975

(d) Rowe *et al* 1974

(e) Plummelle and Vandevyuer 1979

(f) Vekilov and Rusakow 1971

Table 2. Model parameters for the evaluation of phonons.

	$Hg_{1-x}Cd_xTe$	$Hg_{1-x}Zn_xTe$	$Cd_{1-x}Zn_xTe$
α_{10}	1.7736	1.7736	2.005
β_{10}	1.8941	1.8942	2.1514
μ_{10}	0.17188	0.17195	0.1428
α_{20}	1.5281	1.2659	1.7369
β_{20}	1.6434	1.1736	1.6103
μ_{20}	0.10907	0.11151	0.1530
α_{30}	1.8300	1.0503	0.7211
μ_{30}	0.13692	0.13850	0.1478
Z_1	0.7552	0.7552	0.8652
Z_2	0.8652	0.7560	0.7560
θ	-0.3091	-0.7643	-0.2858

(Force constants $\alpha_{10} \dots \mu_{30}$ are in units of $10^4 \text{ dyn. cm}^{-1}$)

Z_1, Z_2 are in units of electronic charge.

θ , dimensionless parameter.

New R and C matrices (compared to the old Varshney *et al*'s R and C matrices) are constructed (given in Appendix I) and a computer program is developed to evaluate phonons for the above mixed systems in this model. Six thousand phonons are generated for the above mixed systems in the first Brillouin zone and classified based

Table 3a. Phonon frequencies along the symmetry directions for $Hg_{1-x}Zn_xTe$.

x	q			ω_{LO1}	ω_{TO1}	ω_{LO2}	ω_{TO2}	ω_{LA}	ω_{TA}
0.2	0.0	0.0	0.0	200.6	176.4	130.9	135.2	—	—
	0.2	0.0	0.0	199.7	176.6	138.8	135.4	33.9	22.6
	0.4	0.0	0.0	196.8	177.3	138.5	136.1	65.7	43.2
	0.6	0.0	0.0	192.2	177.9	137.7	137	93.4	59.9
	0.8	0.0	0.0	186.8	178.3	135.6	137.9	114.9	70.8
	1.0	0.0	0.0	184.2	178.4	131.3	138.2	126.7	74.5
	0.1	0.1	0.1	199.9	176.4	138.9	135.6	67.7	29.8
	0.2	0.2	0.2	197.8	176.6	138.8	135.6	67.7	29.8
	0.3	0.3	0.3	194.2	176.8	138.7	136.1	95.6	41.1
	0.4	0.4	0.4	189.8	177	138.4	136.4	115.8	48.4
0.4	0.5	0.5	0.5	187.6	177	138	136.6	123.8	50.9
	0.0	0.0	0.0	193.6	175.2	140.3	132.7	—	—
	0.2	0.0	0.0	192.8	175.4	140.1	133.1	31.6	20.4
	0.4	0.0	0.0	190.6	175.9	139.4	134.1	61.4	39.0
	0.6	0.0	0.0	187.2	176.4	137.7	135.5	87.4	53.9
	0.8	0.0	0.0	183.5	176.7	134.1	136.6	107.8	63.7
	1.0	0.0	0.0	181.9	176.8	129.8	137.1	118.3	67.0
	0.1	0.1	0.1	193.0	175.3	140.2	132.9	32.7	14.1
	0.2	0.2	0.2	191.4	175.4	139.9	133.4	63.1	26.8
	0.3	0.3	0.3	188.7	175.6	139.1	134.0	89.2	36.8
0.6	0.4	0.4	0.4	185.7	175.7	137.6	134.6	108.2	43.3
	0.5	0.5	0.5	184.2	175.7	136.2	134.8	116.1	45.5
	0.0	0.0	0.0	185.4	172.9	170.4	128.7	—	—
	0.2	0.0	0.0	184.9	173.0	140.1	129.2	29.5	18.5
	0.4	0.0	0.0	183.3	173.3	138.9	130.4	57.3	35.4
	0.6	0.0	0.0	181.0	173.7	136.3	132.0	81.7	48.9
	0.8	0.0	0.0	178.7	173.9	131.6	133.3	101.0	57.0
	1.0	0.0	0.0	177.7	174.0	127.4	133.8	110.4	60.9
	0.1	0.1	0.1	185.0	173.0	140.2	128.9	30.4	12.7
	0.2	0.2	0.2	183.9	173.0	139.5	129.5	58.9	24.2
0.8	0.3	0.3	0.3	182.0	173.1	137.9	130.3	83.3	33.2
	0.4	0.4	0.4	180.1	173.2	135.2	130.9	101.5	39.1
	0.5	0.5	0.5	179.2	173.2	133.1	131.2	109.2	40.1
	0.0	0.0	0.0	175.8	169.3	139.5	123.4	—	—
	0.2	0.0	0.0	175.4	169.3	139.0	123.9	27.4	16.8
	0.4	0.0	0.0	174.6	169.5	137.2	125.3	53.3	32.2
	0.6	0.0	0.0	173.3	169.6	133.7	126.9	76.1	44.7
	0.8	0.0	0.0	172.2	169.7	128.1	128.2	94.1	52.8
	1.0	0.0	0.0	171.8	169.8	123.9	128.7	102.8	55.7
	0.1	0.1	0.1	175.5	169.3	139.2	123.6	28.3	11.5
0.8	0.2	0.2	0.2	174.9	169.3	137.9	124.3	54.8	21.9
	0.3	0.3	0.3	173.9	169.4	135.4	125.1	77.8	30.1
	0.4	0.4	0.4	173.0	169.4	131.6	125.7	95.1	35.4
	0.5	0.5	0.5	172.5	169.4	128.9	125.9	102.5	37.2

(Values are in units of cm^{-1})

on the eigenvectors, the longitudinal, transverse, optic and acoustic modes. These are given in table 3.

Since experimental results on the complete phonon dispersion for the mixed systems are not available, it would be better to see the success of this MRI model by considering

Table 3b. Phonon frequencies along the symmetry directions for $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$.

x	q			ω_{Lo1}	ω_{To1}	ω_{Lo2}	ω_{To2}	ω_{LA}	ω_{TA}
0.2	0.0	0.0	0.0	182.7	168.9	159.6	143.8	0.0	0.0
	0.2	0.0	0.0	181.7	168.9	159.2	144.2	30.9	19.4
	0.4	0.0	0.0	178.8	169	157.5	145.1	60.4	37.2
	0.6	0.0	0.0	175	169.1	153.4	146.2	87.3	51.9
	0.8	0.0	0.0	172.2	169.2	145	146.9	110.3	61.6
	1.0	0.0	0.0	171.3	169.2	135.2	147.2	125.1	65.1
	0.1	0.1	0.1	181.9	168.9	159.2	144	32.4	13.2
	0.2	0.2	0.2	179.5	168.9	157.9	144.4	63	25.1
	0.3	0.3	0.3	176.2	168.9	154.8	144.9	90.5	34.5
	0.4	0.4	0.4	173.4	168.9	148.3	145.3	113.1	40.7
0.4	0.5	0.5	0.5	172.4	168.9	141.6	145.5	125.4	42.8
	0.0	0.0	0.0	190.2	170.7	157.3	147.1	0.0	0.0
	0.2	0.0	0.0	189.1	170.8	157	147.4	32.2	20.7
	0.4	0.0	0.0	185.9	171	155.9	148.2	62.8	39.6
	0.6	0.0	0.0	181.3	171.3	153.1	149.2	90.4	55.1
	0.8	0.0	0.0	177	171.3	147	150	113.5	65.4
	1.0	0.0	0.0	175.2	171.4	139.4	150.3	127	69
	0.1	0.1	0.1	189.4	170.7	157.1	147.2	33.6	14.1
	0.2	0.2	0.2	186.9	170.7	156.2	147.6	65.3	26.9
	0.3	0.3	0.3	183	170.8	154.1	148.1	93.4	37.1
0.6	0.4	0.4	0.4	179	170.8	149.7	148.5	115.9	43.7
	0.5	0.5	0.5	177.2	170.8	145	148.7	127.2	45.9
	0.0	0.0	0.0	196.4	172.5	155.8	149.8	0.0	0.0
	0.2	0.0	0.0	195.3	172.7	155.6	150	33.5	22.1
	0.4	0.0	0.0	192	173.1	154.9	150.6	65.2	42.3
	0.6	0.0	0.0	186.7	173.5	153.1	151.5	93.5	58.8
	0.8	0.0	0.0	181.2	173.7	148.9	152.2	116.6	69.7
	1.0	0.0	0.0	179.3	173.7	147.2	152.4	126.2	72.3
	0.1	0.1	0.1	195.6	172.6	155.6	149.9	34.9	15.2
	0.2	0.2	0.2	193	172.7	155.1	150.2	67.7	28.9
0.8	0.3	0.3	0.3	188.8	172.7	155.1	150.6	96.5	39.9
	0.4	0.4	0.4	183.9	172.8	151.1	150.9	119.9	47
	0.5	0.5	0.5	181.6	172.8	148.1	151.1	129.4	49.4
	0.0	0.0	0.0	201.8	174.5	154.4	151.8	0.0	0.0
	0.2	0.0	0.0	200.7	174.8	154.3	151.9	34.9	23.6
	0.4	0.0	0.0	197.2	175.4	154	152.3	67.7	45.2
	0.6	0.0	0.0	191.6	175.9	153.1	152.8	96.7	62.8
	0.8	0.0	0.0	185.1	176.2	151	153.3	119.6	74.5
	1.0	0.0	0.0	181.7	176.3	148.3	153.4	130.4	78.6
	0.1	0.1	0.1	201	174.6	154.4	151.9	36.3	16.3
0.8	0.2	0.2	0.2	198.4	174.7	154.1	152	70.3	31.1
	0.3	0.3	0.3	193.9	174.9	153.6	152.3	99.8	42.9
	0.4	0.4	0.4	188.4	175	152.3	152.5	122.3	50.6
	0.5	0.5	0.5	185.6	175	150.8	152.4	133	53.2

(Values are in units of cm^{-1})

Table 3c. Phonon frequencies along the symmetry directions for $Hg_{1-x}Cd_xTe$.

x	q			ω_{LO1}	ω_{TO1}	ω_{LO2}	ω_{TO2}	ω_{LA}	ω_{TA}
0.2	0.0	0.0	0.0	153.4	148	136.7	119.4	0.0	0.0
	0.2	0.0	0.0	152.9	148	136.2	119.9	26.2	15.9
	0.4	0.0	0.0	151.5	148.1	134.6	121.1	50.9	30.5
	0.6	0.0	0.0	149.9	148.2	131.1	122.6	73	42.4
	0.8	0.0	0.0	148.6	148.2	125.2	123.7	90.7	50.3
	1.0	0.0	0.0	148.2	148.3	120.5	124.1	99.4	53.1
	0.1	0.1	0.1	153	148	136.4	119.6	27.1	10.8
	0.2	0.2	0.2	151.8	148	135.3	120.2	52.7	20.5
	0.3	0.3	0.3	150.3	148	132.8	120.9	75.1	28.3
	0.4	0.4	0.4	149	148.1	128.4	121.4	92.5	33.3
0.4	0.5	0.5	0.5	148.5	148.1	125.2	121.7	100.2	35
	0.0	0.0	0.0	157.9	147.3	135.6	122	0.0	0.0
	0.2	0.0	0.0	157.1	147.4	135.4	122.4	27	16.5
	0.4	0.0	0.0	154.8	147.6	134.4	123.5	52.6	31.6
	0.6	0.0	0.0	151.5	147.8	131.8	124.7	75.6	43.9
	0.8	0.0	0.0	148.7	147.9	126.6	125.7	94.4	52.1
	1.0	0.0	0.0	147.6	148	121.6	126	104.2	55
	0.1	0.1	0.1	157.3	147.3	135.5	122.2	28.1	11.1
	0.2	0.2	0.2	155.3	147.4	134.8	122.7	54.6	21.2
	0.3	0.3	0.3	152.4	147.5	133.2	123.3	77.9	29.2
0.6	0.4	0.4	0.4	149.5	147.6	129.7	123.8	96.3	34.4
	0.5	0.5	0.5	148.3	147.6	126.5	123.9	104.8	36.2
	0.0	0.0	0.0	162	146	134.4	124.6	0.0	0.0
	0.2	0.0	0.0	160.9	146.1	134.3	124.9	27.9	17
	0.4	0.0	0.0	157.8	146.4	133.7	125.8	54.4	32.7
	0.6	0.0	0.0	152.8	146.8	132.1	126.8	78.3	45.5
	0.8	0.0	0.0	148	147	127.9	127.5	98.3	54
	1.0	0.0	0.0	146	147.1	122.3	127.8	109.5	57.1
	0.1	0.1	0.1	161.2	146	134.3	124.7	29.1	11.5
	0.2	0.2	0.2	158.5	146.2	134	125.1	56.6	21.9
0.8	0.3	0.3	0.3	154.2	146.3	133.1	125.6	80.9	30.2
	0.4	0.4	0.4	149.4	146.4	130.6	126	100.4	35.2
	0.5	0.5	0.5	147.2	146.5	127.5	126.1	109.9	37.3
	0.0	0.0	0.0	165.8	143.8	132.9	127.4	0.0	0.0
	0.2	0.0	0.0	164.5	144	132.8	127.6	28.8	17.6
	0.4	0.0	0.0	160.5	144.5	132.6	128.2	56.2	33.8
	0.6	0.0	0.0	154	145.1	131.9	128.8	81.1	47.2
	0.8	0.0	0.0	146.4	145.5	129.2	129.2	102.4	56.1
	1.0	0.0	0.0	142.7	145.6	122.8	129.4	116.2	59.2
	0.1	0.1	0.1	164.8	143.9	132.9	127.5	30.1	11.9
	0.2	0.2	0.2	161.4	144.1	132.7	127.7	58.6	22.6
	0.3	0.3	0.3	155.8	144.3	132.4	128	84.2	31.2
	0.4	0.4	0.4	148.7	144.5	131.1	128.3	105	36.7
	0.5	0.5	0.5	144.6	144.6	128.5	128.4	115.9	38.6

(Values are in units of cm^{-1})

$x = 0$ and $x = 1$ (end members). That is why dispersion graphs for ZnTe, HgTe and CdTe arrived at from this model for $x = 0.0001$ and $x = 0.9999$ are given in figures 1–3, along with experimental results.

It is important to note that it is not our interest to study the dispersion of ZnTe,

Figure 1. Calculated dispersion curves for $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ and $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ at $x = 0.9999$. $\circ$, $\bullet$ -Experimental results; $\circ$, longitudinal mode; $\bullet$, transverse mode.

Figure 2. Calculated dispersion curves for $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ at $x = 0.0001$ and for $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ at $x = 0.9999$. $\circ$, $\bullet$ -Experimental results; $\circ$, longitudinal mode; $\bullet$, transverse mode.

HgTe and CdTe as there are enough models (Rowe *et al* 1974; Kunc *et al* 1975) available in the literature which could very well explain the experimental results. Since MRI model is attempted for mixed systems, where no experimental results are available, the question of reliability of the model just developed arises and so this type of comparison with end members is done. The agreement with experiment is reasonably good except for TA modes (for end members) and within this limit this MRI model is extended to mixed systems.

The zone centre phonons for $\text{Cd}_{1-x}\text{Hg}_x\text{Te}$ are tabulated in table 4 for different concentrations.

Figure 3. Calculated dispersion curves for $Hg_{1-x}Zn_xTe$ and $Hg_{1-x}Cd_xTe$ at $x=0.0001$. $\circ$, $\bullet$ -Experimental results [41]; $\circ$, longitudinal mode; $\bullet$, transverse mode.

Table 4. Zone centre phonon frequencies for $Cd_{1-x}Hg_xTe$ (in cm^{-1}).

x	L_{01}	T_{01}	L_{02}	T_{02}	L_{01}	T_{01} Expt(b)	L_{02}	T_{02}
0.0	169.4	140	131	131	167.0	140.5	131	131
0.09	167.8	142	132	129	166	141	131	131
0.14	167	143	132	128.3	165	142	132	130
0.24	165	144.3	133.2	126.8	163	142.5	132	128
0.28	164.3	144.8	133.5	126.2	163	141.5	133	128

1 and 2 refer to CdTe-like and HgTe-like frequencies respectively.

(b) Plumelle and Vandevyuer 1976

The advantage of this MRI model is that it could explain the two-mode behaviour also, as seen in figure 4, where the comparison is done with experiment and the REI model.

Thus the MRI model is found to be successful for these systems where no such theoretical works are reported.

2.2 DWF

Because the recent experimental investigations on DWF for these mixed systems are interesting, the complete phonon spectrum which is worked out now can be used to deduce the DWFs for cations and anions at room temperature for various concentrations.

$$\langle u^2 \rangle_k = \frac{\hbar}{NM_k} \sum_{n,qj} \frac{e_a^2(k|qj)(n(qj) + 1/2)}{\omega_j(q)},$$

where the symbols have the usual meanings.

Figure 4. Two mode behaviour of (a) $\text{Zn}_{1-x}\text{Hg}_x\text{Te}$ (●, RE1 model; ▲, experiment), (b) $\text{Cd}_{1-x}\text{Hg}_x\text{Te}$ (●, RE1 model; ▲, experiment), (c) $\text{Zn}_{1-x}\text{Cd}_x\text{Te}$.

Table 5. Calculated values of DWFs at room temperature.

x	$Cd_{1-x}Hg_xTe$		$Zn_{1-x}Hg_xTe$			$Zn_{1-x}Cd_xTe$		
	B_C	B_A	B_C	B_A	B_C Expt(a)	B_A	B_C	B_A
0	1.993	1.546	1.629	1.071	1.358	0.886	1.650	1.071
0.2	1.91	1.546	1.512	1.144	—	—	1.640	1.151
0.25	—	—	1.502	1.165	1.728	1.353	—	—
0.4	1.858	1.550	1.496	1.230	—	—	1.665	1.240
0.5	1.838	1.554	1.510	1.280	1.944	1.701	1.682	1.284
0.6	1.820	1.561	1.534	1.330	—	—	1.700	1.333
0.8	1.800	1.578	1.612	1.454	2.614	1.614	1.760	1.436
0.87	—	—	1.65	1.502	2.822	2.030	—	—
1.0	1.790	1.600	1.726	1.636	—	—	1.830	1.546

(values are in $\text{\AA}^2$) B_C , DWF of cation; B_A , DWF of anion.(a) Baudour *et al* 1989.

The results on DWF are given in table 5 along with experimental results wherever possible.

The present investigations reveal the following:

- (i) In $Zn_{1-x}Hg_xTe$, DWF for cation varies nonmonotonically and for anion monotonically, contradicting the experiment.
- (ii) In $Zn_{1-x}Cd_xTe$ also the trend is the same as that for $Zn_{1-x}Hg_xTe$. But here no experiments are available for comparison.
- (iii) For $Cd_{1-x}Hg_xTe$, the concentration at which the unusual behaviour in DWF occurs could be clearly fixed. At $x = 0.2$, the cation (heavy mass) tries to have higher value of DWF compared to the lower mass. Reid (1984) has reported such anomaly during his experimental investigation on HgTe and a virtual crystal model could not very well fix the concentration (Sadaiyandi 1992).

3. Discussion

Even though the MRI model developed here for the mixed II–VI systems could explain reasonably the experimental phonon dispersion and two-mode behaviour, an averaged property like DWF contradicts the experiments. The reasons may be viewed as follows.

3.1 $Zn_{1-x}Hg_xTe$

Both experiment and theory predict normal behaviour for DWF for ZnTe and anomalous behaviour for HgTe. In HgTe specifically, Hg shows unusual behaviour. Hence when a mixed system of $Zn_{1-x}Hg_xTe$ is formed, it is expected that only the cation ($Zn_{1-x}Hg_x$) behaves nonmonotonically rather than the anion (Te). That is what we have observed from our theory; whereas experiment due to Baudour *et al* predicts the otherway, where a lot of refinements on the experimental data for

anharmonicity, anomalous dispersion and temperature factor are done which might have masked some intricate properties of the system.

3.2 $Zn_{1-x}Cd_xTe$ and $Hg_{1-x}Cd_xTe$

Experimental data on DWF for $Zn_{1-x}Cd_xTe$ are not available for comparison. In $Hg_{1-x}Cd_xTe$, at least the already reported unusual behaviour in DWF is again verified and the concentration could be fixed at $x = 0.2$.

Appendix 1

The nearest-neighbour noncentral short-range interactions give rise to five repulsive force constants $\alpha_1, \beta_1, \alpha_2, \beta_2$ and α_3 , and the second-neighbour central interactions give rise to three force constants μ_1, μ_2 and μ_3 . The subscripts 1, 2 and 3 refer to AC, BC and AB interactions. The effective charge z is the parameter associated with the long-range electrostatic interactions.

The effective charge z and lattice constant a are assumed to vary linearly as

$$z = (1 - x)z_1 + xz_2 \quad (1)$$

and

$$a = (1 - x)a_1 + xa_2, \quad (2)$$

where a_1, z_1 and a_2, z_2 refer to the crystals AC and BC respectively. The force constants are also assumed to vary linearly as

$$\frac{\alpha_1}{\alpha_{10}} = \frac{\beta_1}{\beta_{10}} = \frac{\mu_1}{\mu_{10}} = \frac{\alpha_2}{\alpha_{20}} = \frac{\beta_2}{\beta_{20}} = \frac{\mu_2}{\mu_{20}} = \frac{\alpha_3}{\alpha_{30}} = \frac{\mu_3}{\mu_{30}} = 1 - \theta x, \quad (3)$$

where θ can be thought of as a model parameter. The subscript '0' refers to the force constants when $x = 0$. In the conventional way the generalized equations of motion for the mixed system are set and the short-range interactions are derived. The new form of short-range interaction matrix R , compared to Varshney's (1975), is given below.

$$R_{xx}(AA) = 4(\alpha_1 + (1 - x)\mu_1(2 - C_{xyz}) + x(\alpha_3 + 2\mu_3))$$

$$R_{xx}(BB) = 4(\alpha_2 + x\mu_2(2 - C_{xyz}) + (1 - x)(\alpha_3 + 2\mu_3))$$

$$R_{xx}(CC) = 4(1 - x)(\alpha_1 + \mu_1(2 - C_{xyz}) + x(\alpha_2 + \mu_2(2 - C_{xyz})))$$

$$R_{xx}(AB) = -4(\alpha_1(1 - x))^{1/2}(\alpha_3 + \mu_3 C_{xyz})$$

$$R_{xy}(AA) = 4(1 - x)\mu_1 \sin \pi q_x \cdot \sin \pi q_y$$

$$R_{xy}(BB) = \frac{x}{(1 - x)} \frac{\mu_2}{\mu_1} R_{xy}(AA)$$

$$R_{xy}(CC) = R_{xy}(AA) + R_{xy}(BB)$$

$$R_{xy}(AB) = \frac{x^{1/2}}{(1 - x)^{1/2}} \frac{\mu_3}{\mu_1} R_{xy}(AA)$$

$$\begin{aligned}
R_{xx}(AC) &= -(1-x)^{1/2} \alpha_1 (a_1 + a_2 + a_3 + a_4) \\
R_{xx}(BC) &= \frac{x^{1/2}}{(1-x)^{1/2}} \frac{\alpha_2}{\alpha_1} R_{xx}(AC) \\
R_{xy}(AC) &= -(1-x)^{1/2} \beta_1 (a_1 + a_2 - a_3 - a_4) \\
R_{xy}(BC) &= \frac{x^{1/2}}{(1-x)^{1/2}} \frac{\beta_2}{\beta_1} R_{xx}(AC) \\
R_{xz}(AC) &= -(1-x)^{1/2} \beta_1 (a_1 + a_2 + a_3 - a_4) \\
R_{xz}(BC) &= \frac{x^{1/2}}{(1-x)^{1/2}} \frac{\beta_2}{\beta_1} R_{xz}(AC) \\
R_{yz}(AC) &= -(1-x)^{1/2} \beta_1 (a_1 - a_2 - a_3 + a_4) \\
R_{yz}(BC) &= \frac{x^{1/2}}{(1-x)^{1/2}} \frac{\beta_2}{\beta_1} R_{yz}(AC), \tag{4}
\end{aligned}$$

where $C_{xyz} = \cos \pi q_y + \cos \pi q_z \cos \pi q_x$

$$\begin{aligned}
a_1 &= \exp\left(i \frac{\pi}{q} (q_x + q_y + q_z)\right) \\
a_2 &= \exp\left(i \frac{\pi}{q} (q_z - q_x - q_y)\right) \\
a_3 &= \exp\left(i \frac{\pi}{q} (q_y - q_z - q_x)\right) \\
a_4 &= \exp\left(i \frac{\pi}{q} (q_x - q_y - q_z)\right).
\end{aligned}$$

Similarly Coulomb interactions are obtained by suitably modifying the C matrix given by Woods *et al* (1960) and the modified C matrix at $q \rightarrow 0$ is given as

$$\begin{aligned}
C_{xx}(AA) &= -2C_{yy}(AA) = -2C_{zz}(AA) = (1-x)C_z \\
C_{xx}(BB) &= -2C_{yy}(BB) = -2C_{zz}(BB) = xC_z \\
C_{xx}(CC) &= -2C_{yy}(CC) = -2C_{zz}(CC) = C_z \\
C_{xx}(AC) &= -2C_{yy}(AC) = -2C_{zz}(AC) = -(1-x)^{1/2} C_z \\
C_{xx}(BC) &= -2C_{yy}(BC) = -2C_{zz}(BC) = -x^{1/2} C_z \\
C_{xx}(AB) &= -2C_{yy}(AB) = -2C_{zz}(AB) = (x(1-x))^{1/2} C_z, \tag{5}
\end{aligned}$$

where

$$C_z = \frac{8\pi z^2 e^2}{3 \cdot V},$$

and V , the volume, $= a^3/4$ for zinc blende structure.

The model parameters are worked out from the equations (21) to (34) of Varshney *et al* (1975). There are eleven parameters to be evaluated from the elastic constants, zone centre frequencies and impurity mode frequencies of the end members. The input data for the evaluation of model parameters are given in table 1. $\alpha_{10}, z_1, \alpha_{20}, z_2$ and θ are evaluated from the equations (24) to (26) and (28) to (30) of Varshney *et al* unambiguously. Since there is an imbalance between the number of equations available and the number of parameters to be evaluated, the parameters $\beta_{10}, \mu_{10}, \beta_{20}$ and μ_{20} are calculated by a least-squares method. This is done using an IMSL subroutine on CYBER 180/830 A. The remaining parameters α_{30} and μ_{30} are calculated from equations (31) and (34) of Varshney *et al* respectively. The whole set of parameters thus evaluated for $\text{Zn}_{1-x}\text{Hg}_x\text{Te}$, $\text{Zn}_{1-x}\text{Cd}_x\text{Te}$ and $\text{Cd}_{1-x}\text{Hg}_x\text{Te}$ are tabulated in table 2.

References

- Barker A S and Sievers A J 1975 *Rev. Mod. Phys.* **47** Suppl. 12
 Baudour J L, Granger M M, Toupet L, Granger R and Triboulet R 1989 *J. Phys. Chem. Solids* **50** 30
 Gaur S P *et al* 1971 *J. Phys. Chem. Solids* **32** 2737
 Kunc K, Balkanski M and Nusimovici M A 1975a *Phys. Status Solidi* **b72** 229
 Plummelle P and Vandevyuer M 1979 *Phys. Status Solidi* **b92** 945
 Reid J S 1983 *Acta Crystallogr.* **A39** 1
 Rowe J M, Nicklow R M, Price D L and Zanio K 1974 *Phys. Rev.* **B10** 617
 Sadaiyandi K 1992 *Lattice dynamical investigations on some semiconducting crystals*, Ph. D. Thesis, Madurai Kamaraj University, Madurai
 Varshney S C, Vetelion J F, Mitra S S and Chang I F 1975 *Phys. Rev.* **B12** 5912
 Vegelato S N, Wehe D and King J S 1974 *J. Chem. Phys.* **60** 3613
 Vekilov Yu Kh and Rusakow A P 1971 *Sov. Phys. Solid State* **13** 956
 Woods A D B, Cochran W and Brockhouse B N 1960 *Phys. Rev.* **119** 980