J. Indian Chem. Soc.,
Vol. 87, March 2010, pp. 345-353

NOTE

Theoretical evaluation of crystalline state properties of chalcogenide crystals with sodium chloride structure

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Manuscript received 16 October 2008, revised 3 June 2009, accepted 3 June 2009

Abstract : Hellmann and Ali-Hasan forms of repulsive potential functions have been applied to compute the values of cohesive energy, atomization energy, force constant, IR absorption frequency, Debye temperature, Grüneisen parameter, Anderson-Grüneisen parameter and Moelwyn-Hughes parameter for 45 chalcogenide crystals of NaCl-structure. The results are reported here. Calculations are also performed for the estimation of first order volume dependence of Grüneisen parameter commonly known as second Grüneisen parameter using expressions of higher order derivatives of interaction potential within the frame-work of Dugdale and MacDonald theory. The high pressure behaviour of these crystals have also been studied.

Keywords : Crystalline state properties, Grüneisen parameter, second Grüneisen parameter.

Introduction

The nature of bonding in ionic crystals has been the centre of attraction for theoretical as well as experimental physicists and chemists as it plays a vital role in solid state physics. Several attempts have been made to understand the nature of interaction between the atoms of an ionic crystal and hence to decide the form of interaction potential for such a crystal. Once the reliable form of interaction potential is known, it is possible to study the crystalline state properties of chalcogenide crystal. The crystal state properties of chalcogenides have been studied by several workers. But these investigators employed the interaction models[1-4] with repulsive parts that are either inverse power functions or exponential functions or phenomenological in nature. But none of these are capable enough of explaining all the observed macroscopic properties of diatomic crystals. The search for the interaction potential function satisfying the essential requirements of ideal potential function[5] continues.

In the present communication we have used the Hellmann[6] and Ali-Hasan[7] short-range repulsive potential to evaluate the crystalline state properties of chalcogenide crystals. The reason for selecting these models lies in their suitability[8] of evaluating their state properties as well as molecular state properties. Moreover, these potentials fulfill the fundamental physical requirements of an ideal potential.

Method of analysis :

Crystal energy : The crystal lattice energy per ion pair can be expressed as

$$\Phi(r) = \Phi_e + \Phi_v + \Phi_{SR} \quad (1)$$

Here Φ_e is the long-range electrostatic coulomb energy with Madelung constant A. It is given by

$$\Phi_e = -Az_1 z_2 e^2/r \quad (2)$$

where z_1e and z_2e are the electrostatic charges on the ion pairs and r is the interionic separation.

The second term, Φ_v, on the R.H.S. of the eq. (1) represents the van der Waals energy expressed as

$$\Phi_v = -C/r^6 - D/r^8 \quad (3)$$

where C and D are van der Waals (vdw) dipole-dipole and dipole quadrupole co-efficients and are given by

$$C = S_{+-}c_{+-} + S_{++}c_{++} + S_{--}c_{--}$$

and

$$D = T_{+-}d_{+-} + T_{++}d_{++} + T_{--}d_{--} \quad (4)$$

Lattice sums S_{ij} and T_{ij} have been taken from Tosi[9] and vdw co-efficients c_{ij} and d_{ij} are taken from Shankar, Singh and Agarwal[10].

The last term Φ_{SR} on the R.H.S. of the eq. (1) is expressed as

$$\Phi_{SR} = S/r^m \exp(-\lambda r^n) \quad (5)$$

where S and λ are potential parameters evaluated by applying the following crystal stability conditions :

$$\Phi'(r_0) = 0$$

and

$$\Phi''(r_0) = 9kr_0/\beta \tag{6}$$

where k = crystals structure constant and β = isothermal compressibility.

In the above equations r_0 is the equilibrium interionic separation in the lattice and the primes denote derivatives with respect to r.

The application of the above conditions to the potentials function yields the expression for the potential parameters :

$$S = \frac{r^m\,[Az_1 z_2 e^2/r_0 + 6C/r_0^6 + 8D/r_0^8]}{\exp(-\lambda r^n)\,(m + n\lambda r^n)} \tag{7}$$

and

$$\lambda = \frac{X + n - 2m - 1 + [(X + n - 2m - 1)^2 - \{4m\,(M + 1)\} - X]^{1/2}}{r^n\, 2n} \tag{8}$$

where

$$X = \frac{9kr_0^3 + 2Az_1 z_2 e^2/r_0 + 42C/r_0^6 + 72D/r_0^8}{Az_1 z_2 e^2/r_0 + 6C/r_0^6 + 8D/r_0^8} \tag{9}$$

where

$z_1 = z_2 = 2$ for alkali earth chalcogenide crystals

and

$m = 1$, $n = 1$ for Helmann model

$m = 2$, $n = 3/2$ for Ali-Hasan model

The last term Φ_{SR} of the eq. (1) is the short-range overlap repulsive energy dominant in diatomic crystals. The short-range repulsive potential perturbs the spherically symmetric closed shell of an ion in a lattice as the ions are brought closer so that outer electron shells began to overlap. An additional characteristic repulsive force becomes operative resulting from the overlapping of the ions. This repulsive force opposes the Coulumbian attractive force operating between the positive and the negative ions and causes them to come to equilibrium at finite value of the interionic distance (r_0). This repulsive force in an ion becomes dominant at a very short distance, so it is known as short-range repulsive potential (SRRP). The exact form of SRRP in literature is still lacking.

Cohesive energy :

The cohesive energy W per mole is related to the interaction potential energy function Φ (r) by

$$W = -N\,\Phi(r) \tag{10}$$

where N is Avogadro's number.

Atomization energy :

The atomization energy of diatomic crystals is of much interest since it gives a better idea of the stability of the crystals than the cohesive energy. Only a few experimental and theoretical attempts have been made to estimate E_a for some of these crystals[11]. The values of E_a for a particular ionic crystal AB may also be computed form the interaction potential energy function by the relation,

$$E_a = W - E - I \tag{11}$$

where E is the electron affinity for forming B^{2-} ions and I is the ionisation energy to produce A^{2+} ions. In the present calculation the values of I have been taken from Massey[12] and those of E from Ladd and Lee[13].

Force constant (f), IR absorption frequency (ν_0) and Debye temperature (θ_D) :

The force constant f is defined[23] as

$$f = 1/3\,[\Psi''(r_0) + 2r_0^{-1}\,\Psi'(r_0)] \tag{12}$$

where Ψ (r) is the non-Coulumbic part of Φ (r) and r_0 is the equilibrium interionic distance in crystalline states. Its values are taken from Sinha *et al.*[14].

The IR absorption frequency (ν_0) is given by[23]

$$\nu_0 = 1/2\pi(f/m)^{1/2}$$

where m is the reduced mass.

Once the value of ν_0 is obtained, the Debye temperature θ_D can be calculated from the relation[23],

$$\theta_D = h\,\nu_0/k$$

where h is the Planck's constant and k is the Boltzmann constant.

Grüneisen parameter, Anderson-Grüneisen parameter and Moelwvn-Hughes parameter :

The Grüneisen parameter γ is the first significant measure of the anharmonicity in solids[23]. It is related to Φ (r) by

$$\gamma = (-1/6r_0)\Phi'''(r_0)/\Phi''(r_0) \tag{13}$$

where $\Phi''(r)$ and $\Phi'''(r)$ refer to the second and third derivatives of $\Phi(r)$.

Anderson-Grüneisen parameter :

Anderson-Grüneisen parameters δ have been computed using chang's expression[15] connecting γ and δ which was derived on the basis of Dugdale and MacDonald formula[16] relating γ to the change of compressibility with volume.

The values of the Moelwyn-Hughes parameter C_1 have been computed for the potential $\Phi(r)$ using the relation[23]

$$C_1 = 1 - (r_0^3\, \beta/27V)\, \Phi'''(r_0) \qquad (14)$$

where β is the compressibility of the crystals.

Second Grüneisen parameter :

The first order volume dependence of the Grüneisen parameter commonly known as the second Grüneisen parameter is fundamental to the study of many basic phenomena in solids. It is an additional measure of the anharmonicity in solids. γ and q can be used to make predictions of a variety of physical properties such as the equation of state of a material and are related to thermodynamic properties. These are also important in the study of thermo-elastic properties in terms of shock-waves. The latter property is especially relevant to the study of the geophysics of the earth.

In general, the Grüneisen parameter is a function of both temperature and volume. The temperature of Grüneisen parameter for a large number of diatomic crystals can be fairly determined either experimentally or theoretically. However, the explicit dependence of Grüneisen parameter on volume is not known accurately. Davies and Parker[17] were the first to define second Grüneisen parameter q as

$$q = [\delta \ln \gamma / \delta \ln \gamma]_T \qquad (15)$$

Basset *et al.*[18] proposed an expression for q using thermodynamic relations.

In this communication an attempt has been made to calculate q for chalcogenide crystals using Hellman and Ali-Hasan forms of interaction models within the frame work of Dugdale and MacDonald theory (DM).

Grüneisen parameter (γ) based on DM theory valid at all pressures may be expressed as

$$\gamma = -1 - V/2\, (\partial^2 P/\partial V^2 - 10P/9V^2)\, (\partial P/\partial V + 2P/3V)^{-1}. \qquad (16)$$

The second Grüneisen parameter (q) derived from eq. (1) is written as

$$\begin{aligned} q = -V/2\gamma[&(\partial^2 P/\partial V^2 - 10P/9V^2)\\ &(\partial P/\partial V + 2P/3V)^{-1} + (\partial P/\partial V + 2P/3V)\\ &(\partial^3 P/\partial V^3 - 10/V^2\, \partial P/\partial V + 20P/V^3)\\ &- V(\partial^2 P/\partial V^2 - 10P/9V^2)\, (\partial P/\partial V + 2P/3V)^{-2}\\ &(\partial^2 P/\partial V^2 + 2/3V\, \partial P/\partial V - 2/3\, P/V^2)] \end{aligned} \qquad (17)$$

Hilderbrand equation of state[19] can be used to express γ and q in terms of derivatives of potential energy function.

For crystals with NaCl-structure

$$P = -\partial\Phi/\partial V = -1/6\, r^2\, \Phi'(r) \qquad (18)$$

$$\partial P/\partial V = -1/36\, r^4\, (\Phi'' - 2/r\, \Phi'(r)) \qquad (19)$$

$$\partial^2 P/\partial V^2 = -1/216\, r^6\, [\Phi'''\, 6/r\, \Phi'' + 10/r^2\, \Phi'] \qquad (20)$$

$$\begin{aligned} \partial^2 P/\partial V^3 = -1/129\, r^8\, [&\Phi'''' - 12/r\, \Phi''' +\\ &52/r^2\, \Phi'' - 80/r^3 \Phi'\,] \end{aligned} \qquad (21)$$

where the primes denote the derivatives of $\Phi(r)$ with respect to interionic separation.

Equation of state of earth chalcogenides :

The high pressure behaviour of these crystals is investigated by determining the compression values of these crystals by using Murnaghan logarithmic equation of state expressed as

$$V/V_0 = \exp[(-1/B'_0)\, \log_e \{(PB'_0/B_0) + 1\}] \qquad (22)$$

where B_0 and B'_0 are isothermal bulk modulus and its pressure derivatives, both referred to zero pressure[24]. The high pressure behaviour of these crystals have been shown below in Fig. 1.

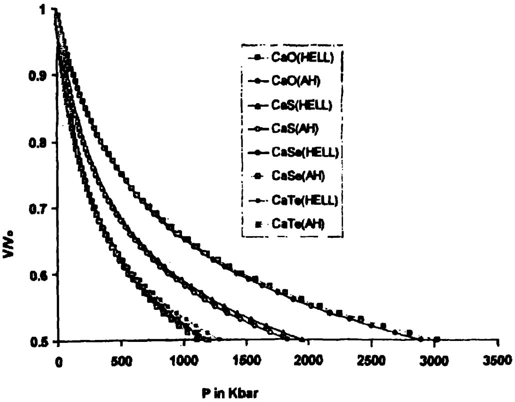

Fig. 1. Compression curves V/V_0 pressure P (KBar) for chalcogenide crystals based on our interionic potential models.

Results and discussion

The latest information on chalcogenide crystals is far from complete but this work tries to add a little to the knowledge of these crystals by predicting several crystalline state properties such as cohesive energy (*W*), atomization energy (E_a), force constant, IR absorption frequency (ν_0), Debye temperature, Anderson-Grüneisen parameter (δ), Moelwyn-Hughes parameter (C_1) and second Grüneisen parameter (q) respectively.

Hellmann and Ali-Hasan forms of short-range repulsive potential have been used to compute *W* and E_a of chalcogenide crystals and their values are listed in Table 1. It is found that the cohesive energy of a AO > AS > ASe > ATe for both the models. The earlier works by Waddington[20], Rossini *et al.*[21] and Thakur[22] have also obtained the values of *W* but their values are not satisfactory as they have not included the van der Waals terms.

The present values of E_a compare well with the experimental values. It is also compared to the values calculated by Thakur[1]. It is observed that the inclusion of van der Waals terms improves the results expectedly and given the better agreement as this match was missing in earlier calculation. Out of the two Hellmann and Ali-Hasan models, the latter presents a better result.

Table 1. Calculated properties of alkali earth chalcogenide crystals

Cohesive energy (kJ mol^{-1}), atomization energy (kJ mol^{-1}) and Experimental values

Crystals	*W*			E_a			
	(Hell)	(AH)	(Expt.[1])	(Hell)	(AH)	(Expt.[1])	(Calcd.[1])
Oxides :							
MgO	3790.60	3817.15	3899.5	883.60	910.15	1000	753
CaO	3362.09	3386.32	3510.4	909.00	933.33	1058.6	907
TiO	3725.74	3765.08	3882.8	1050.74	1090.02		995
MnO	3674.84	3704.94	3815.8	729.84	759.94	912.1	545
FeO	3769.63	3803.44	3924.6	729.63	691.04		560
CoO	3771.58	3806.04	3995.7	656.58	691.04		495
NiO	3822.43	3861.19	4083.6	615.43	654.19		483
SrO	3190.66	3213.02	3330.5	861.86	884.02	1000	831
ZrO	3505.87	3537.74		862.87	894.74		837
NbO	3673.00	3718.23		909.01	954.23		896
CdO	3890.15	3421.11	3782.3	180.15	211.11	615.1	210
BaO	3041.49	3062.14	3288.6	857.49	878.14	979.1	976
TaO	3559.33	3613.22		523.33	577.22		464
UO	3380.75	34420.18					
Sulphides :							
MgS	3221.68	3247.46	3748.9	612.38	637.26	774.0	746
CaS	2908.45	2930.58	3196.6	752.95	775.08	920.5	802
MnS	3104.66	3135.64	3351.4	457.16	488.19	761.5	746
SrS	2839.77	2861.89	3012.5	808.27	830.39	895.4	780
ZrS	3135.15	3169.58		789.65	824.08		770
BaS	2637.90	2657.50	2841	749.90	769.56	895.4	782
LaS	2919.90	2945.08		854.90	880.08		825
CeS	2944.67	2917.35		710.67	737.35		662
PhS	2843.62	2876.46	3092	256.62	289.46	564.8	153
ThS	3015.50	3051.92					
US	3089.57	3133.91					
Selenides :							
MgSe	2959.60	29985.18	3343	278.10	303.68	627.6	334

Table-1 (contd.)

CaSe	2747.14	2770.91	3033.4	519.64	543.41	702.9	636
MnSe	2991.59	3023.56	3305.4	272.09	304.06		297
SrSe	2646.31	2668.63	2903.7	542.81	565.13	698.7	625
SnSe	2757.21	2784.68		149.21	176.68		202
BaSe	2512.16	2533.49	2761.4	550.16	571.49	690.4	668
LaSe	2754.25	2782.09		617.25	645.04		662
CeSe	2779.61	2809.44		473.61	503.44		524
PbSe	2686.35	2723.98		30.35	67.98		224
ThSe	2822.79	2863.66					
USe	2846.60	2892.58					
Tellurides :							
CaTe	2833.92	2652.42	2840.9	490.42	512.92		547
SrTe	2383.53	2406.17	2790.7	364.03	386.67		653
SnTe	2702.00	2729.53		178.01	205.53		173
BaTe	2428.16	2448.23	2631.7	550.16	570.23		622
LaTe	2681.47	2708.08		628.47	655.08		610
CeTe	2702.00	2730.17		480.00	508.17		364
PbTe	2634.38	2670.05		63.38	99.05		79
BiTe	2683.35	2713.88					
UTe	2790.58	2832.25					

Table 2 lists the calculated values of f, ν_0 and θ_D and no comparison can be made the agreement between the theoretical and experimental values as the experimental values are not available in the literature. The present calculation shows that van der Waals energy is important for heavier crystals. It is observed that the two models give almost identical results of f, ν_0 and θ_D. In our earlier work[25] we observe that Varshini-Shukla model has distinct advantage over other models.

The calculated values of γ, δ, C_1 and q have been listed in Table 3. There is no experimental data to draw comparison. But the present results indicate that γ de-

Table 2. Calculated properties of alkali earth chalcogenide crystals

Force constant f (Nm^{-1}), IR absorption frequency ν_0 (10^{12} HZ) and Debye temperature θ_D (K)

Crystals	f				θ_D	
	(Present)	(Calcd.[22])	(Present)	(Calcd.[22])	(Present)	(Calcd.[22])
Oxides :						
MgO	18.16	21.5	20.89	18.4	871.84	886
CaC	14.21	16.7	15.24	14.9	682.47	716
TiO	13.56	21.8	14.57	16.7	651.30	800
MnO	15.65	19.3	20.03	15.4	751.26	741
FeO	15.63	20.7	20.06	15.9	750.36	765
CoO	15.32	21.0	19.50	16.1	735.60	775
NiO	14.91	21.9	18.41	15.6	716.21	751
SiO	12.56	14.6	14.10	12.8	603.20	616
ZrO	13.41	18.1	16.12	14.2	643.79	683
NbO	11.42	21.5	11.76	15.6	548.52	746
CdO	12.07	17.5	13.51	13.8	579.89	662
BaO	11.84	11.6	13.26	12.5	568.45	599

Table-2 (contd.)

TaO	10.30	19.5	10.30	14.7	494.68	707
UO	12.20	16.0	14.73	12.8	585.80	612
Sulphides :						
MgS	12.30	14.4	13.69	12.6	590.49	605
CaS	9.53	12.1	10.65	6.4	457.59	309
MnS	9.00	19.3	10.82	12.1	432.37	579
SrS	8.12	10.9	10.21	8.4	390.00	404
ZrS	8.56	14.1	11.48	9.5	411.07	457
BaS	7.08	9.7	8.61	7.4	340.28	355
LaS	8.27	11.5	11.74	8.2	397.11	394
CeS	12.30	11.8	11.77	8.3	590.89	398
PhS	7.18	11.2	9.43	6.8	344.63	327
ThS	7.93	12.2	11.69	8.1	380.63	390
US	7.68	13.0	10.98	8.4	368.83	402
Selenides :						
MgSe	8.90	13.2	9.73	10.4	427.47	499
CaSe	6.75	11.2	8.00	8.0	324.06	385
MnSe	6.73	13.2	9.68	7.9	322.98	378
SrSe	5.27	10.2	7.68	6.1	253.12	294
SnSe	5.17	10.9	8.45	5.1	248.07	246
BaSe	4.50	9.1	6.71	5.3	216.20	253
LaSe	5.06	11.0	8.58	5.7	243.02	274
CeSe	5.04	11.0	8.47	5.8	241.96	277
PbSe	4.00	10.5	6.11	5.3	192.24	254
ThSe	4.39	11.4	7.50	5.4	210.86	261
USe	4.11	11.9	6.61	5.5	197.24	265
Tellurides :						
CaTe	6.28	9.9	7.95	6.3	301.69	301
SrTe	3.64	9.5	4.56	5.3	174.98	253
SnTe	4.63	10.0	8.82	5.0	222.26	239
BaTe	3.92	8.2	6.71	4.4	188.21	209
LaTe	4.50	9.7	8.98	4.7	216.13	226
CeTe	4.51	9.8	8.97	4.7	216.59	227
PbTe	3.68	9.5	7.16	4.3	176.81	206
BiTe	4.10	9.5	8.91	4.3	197.05	205
UTe	3.94	10.4	8.50	4.4	189.02	210

Table 3. Calculated properties of alkali earth chalcogenide crystals

Values of Grüneisen parameter (γ : dimensionless), Anderson-Grüneisen parameter (δ : dimensionless), Moelwyn-Hughes parameter (C_1) and second Grüneisen parameter (q : dimensionless)

Crystals	γ			δ			C_1			q	
	(Hell)	(AH)	(Calcd.[1])	(Hell)	(AH)	(Calcd.[1])	(Hell)	(AH)	(Calcd.[1])	(Hell)	(AH)
Oxides :											
MgO	1.17	1.13	1.61	2.34	2.26	3.22	3.34	3.26	4.20	0.77	0.80
CaO	1.22	1.17	1.62	2.44	2.35	3.24	3.44	3.35	4.24	0.79	0.84
TiO	0.82	0.92	1.59	1.64	1.84	3.18	1.97	1.83	4.18	5.30	6.62
MnO	1.19	1.13	1.68	2.38	2.26	3.36	3.39	3.26	4.31	0.96	1.05

Table-3 (contd.)

FeO	1.06	0.99	1.64	2.11	1.98	3.28	3.12	2.98	4.28	1.21	1.37
CoO	1.01	0.94	1.63	2.01	1.88	3.26	3.01	2.88	4.26	1.32	1.50
NiO	0.80	0.73	1.60	1.60	1.46	3.20	2.60	2.46	4.20	2.18	2.58
SrO	1.33	1.28	1.76	2.66	2.55	3.52	3.66	3.55	4.52	0.76	0.82
ZrO	1.05	0.99	1.55	2.10	1.97	3.10	3.10	2.97	4.10	1.22	1.38
NbO	1.11	1.21	1.61	2.22	2.42	3.22	0.98	0.78	4.22	1.22	1.32
CdO	0.94	0.87	1.58	1.87	1.76	3.16	2.88	2.76	4.16	1.46	1.62
BaO	1.45	1.38	1.78	2.89	2.76	3.56	3.89	3.76	4.56	0 77	0 84
TaO	0.86	1.01	1.69	1.72	2.02	3.38	0.43	0.10	4 38	1.15	1.19
UO	1.01	0.90	1.66	2.01	1.80	3.32	3.01	2 80	4.32	1.08	2.12
Sulphides :											
MgS	1.22	1.16	1.76	2.44	2.33	3.52	3.45	3.32	4.52	0.89	0.98
CaS	1.31	1.23	1.74	2.62	2.49	3.48	3.62	3.49	4.48	0.83	0.92
MnS	0.97	0.89	1.69	1.94	1.79	3.40	2.94	2.79	4.40	1.52	1.79
SrS	1.35	1.28	1.86	2.69	2.56	3.72	3.69	3.56	4.72	0.84	0.94
ZrS	0.98	0.89	1.78	1.97	1.78	3.56	2.97	2.78	4.56	1.66	2.04
BaS	1.43	1.36	1.99	2.85	2.71	3.98	3.85	3.71	4.98	0.81	0.91
LaS	1.41	1.33	1.79	2.82	2.65	3.58	33.82	3.65	4.58	0 90	1.04
CeS	1.37	1.28	1.77	2.74	2.56	3.59	3.73	3.56	4.54	0.96	1.10
PhS	1.13	1.03	1.62	2.27	2.05	3.24	3.27	3.05	4.24	1.39	1.73
ThS	1.19	1.07	1.73	2.37	2.13	3.46	3.37	3.13	4.46	1.36	1.72
US	0.89	0.75	1.86	1.78	1.50	3.72	2.78	2.50	4.72	2.47	3.47
Selenides :											
MgSe	1.08	1.02	1.85	2.17	2.04	3.70	3.16	3.05	4.70	1.08	1.19
CaSe	1.12	1.05	1.82	2.24	2.12	3.64	3.24	3.12	4.64	1.04	1.15
MnSe	0.95	0.86	1.85	1.89	1.72	3.70	2.89	2.73	4 70	1.68	2.04
SrSe	1.23	1.16	1.93	2.46	2.32	3.86	3.46	3.32	4.86	0.93	1.05
SnSe	1.15	1.06	1.86	2.29	2.12	3.72	3.29	3.12	4.72	1.13	1 40
BaSe	1.26	1.19	1.87	2.52	2.37	3.74	3.52	3.38	4.74	0.92	1.04
LaSe	1.17	1.08	1.87	2.34	2.16	3.74	3.35	3.17	4.74	1.17	1.40
CeSe	1.09	0.99	1.85	2.18	1.99	3.70	3.18	2.99	4.70	1.36	1.65
PbSe	0.58	0.45	2.02	1.16	0.89	4.04	2.16	1.89	5.04	4.87	7.29
ThSe	0.68	0.54	1.80	1.36	1.08	3.60	2.38	2.08	4.60	3.89	5.76
USe	0.28	0.45	1.76	0.56	0.90	3.52	1.56	1.23	4.52	1.45	1.48
Tellurides :											
CaTe	1.29	1.22	1.98	2.59	2.45	3.96	3.59	3.45	4.96	0.91	1.04
SrTe	0.89	0.82	1.84	1.77	1.65	3.68	2.77	2.65	4.68	1.61	1.83
SnTe	1.30	1.21	1.96	2.61	2.41	3.92	3.61	3.41	4.92	1.06	1.26
BaTe	1.41	1.33	2.02	2.82	2.66	4.04	3.82	3.66	5.02	0.87	0.97
LaTe	1.37	1.28	2.00	2.75	2.55	3.99	3.75	3.55	4.94	1.00	1.18
CeTe	1.33	1.23	1.74	2.66	2.45	3.48	3.66	3.45	4.48	1.05	1.27
PbTe	1.02	0.89	2.01	2.03	1.77	4.02	3.03	2.77	5.02	1.85	2.46
BiTe	1.36	1.22	2.02	2.67	2.45	4.04	3.67	3.45	5.04	1.11	1.37
UTe	0.98	0.84	1.94	1.97	1.67	3.82	2.97	2.67	4.82	2.11	2.95

pends upon the specific volume since the values tend to increase as we move from oxides to tellurides.

We have investigated the high pressure behaviour of these crystals. The equation works well up to very high pressure. The compression curves are given in Fig. 1. The graphical behaviour of force constant and cohesive energy, reduced mass and Debye temperature, logarithm of specific volume and logarithm Debye temperature, reduced mass and IR frequency are shown in Figs. 2-5 respectively. The experimental data for the compressions of chalcogenide crystals are not available in the literature and hence it is not possible to draw experimental curves for these crystals.

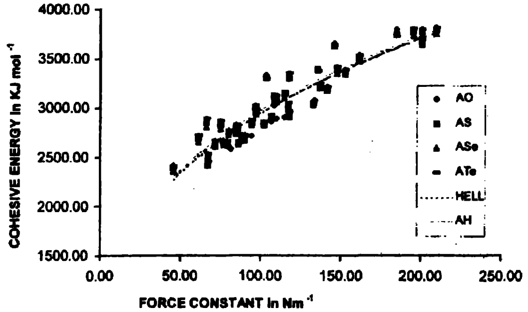

Fig. 2. A plot of force constant versus cohesive energy for alkali earth chalcogenides.

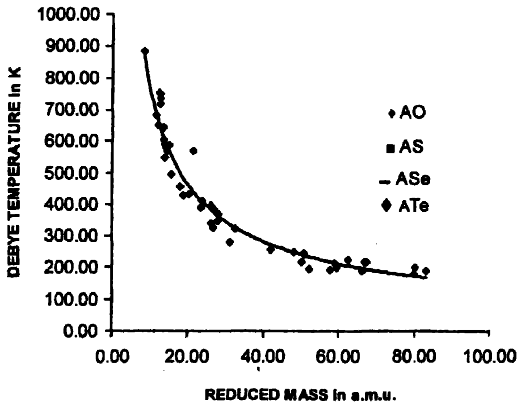

Fig. 3. A plot of reduced mass versus Debye temperature for alkali earth chalcogenide crystals.

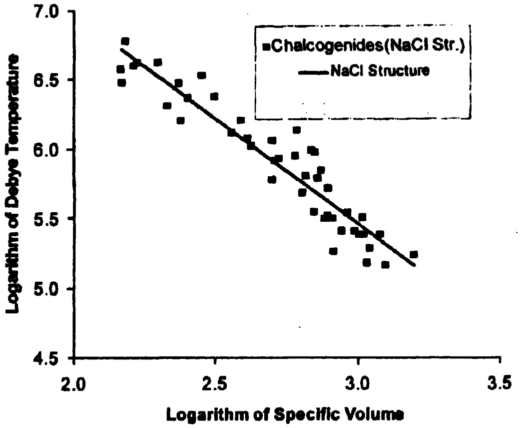

Fig. 4. A plot of logarithm of specific volume versus logarithm of Debye temperature for alkali earth chalcogenide crystals.

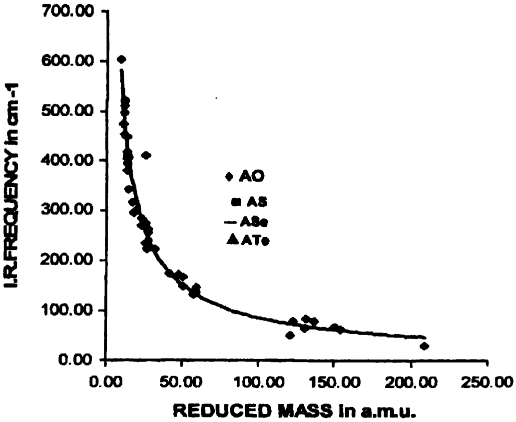

Fig. 5. A plot of reduced mass versus IR frequency of alkali earth chalcogenide crystals.

Conclusion :

Hellmann and Ali-Hasan forms of interaction potential have been applied to get different crystalline state properties of chalcogenide crystals. The latter model gives encouraging result and may prove useful for further computation of the properties of such crystals.

Acknowledgement

We are extremely thankful to Prof. Md. M. M. Hasan for his keen interest in the completion of this work. We are highly grateful to the learner referee for providing useful suggestions.

References

1. K. P. Thakur, *Aust. J. Phys.*, 1977, **30**, 323.
2. R. Rydberg, *Z. Phys.*, 1931, **73**, 376.
3. J. Shankar and M. Kumar, *Phys. Status Solidi (b)*, 1987, **142**, 325.
4. R. Narayan and S. Ramaseshan, *J. Phys. Chem. Solids*, 1976, **37**, 395.
5. Y. P. Varshini and R. C. Shukla, *Rev. Mod. Phys.*, 1963, **35**, 130.
6. H. Hellamann, *Acta Phys. Chem. (USSR)*, 1934, **1**, 113.
7. Y. P. Varshini and R. P. C. Shukla, *J. Chem. Phys. (USA)*, 1978, **69**, 670.
8. J. Mandal and B. Ghatak, *J. Indian Chem. Soc.*, 2007, **84** 145.
9. M. P. Tosi, *Solid State Phys.*, 1964, **16**, 1.
10. J. Shankar G. G. Agrawal and R. P. Singh, *J. Chem. Phys. (USA)*, 1978, **69**, 670.
11. R. T. Sanderson, "Inorganic Chemistry", Reinhold, New York, 1967.
12. A. G. Massey, "The Typical Elements", Penguin, Middlesex, 1972.
13. M. F. C. Ladd and W. H. Lee, *Prog. Solid State Chem.*, 1965, **1**, 17.
14. S. P. Sinha and K. P. Thakur, *Indian J. Pure Appl. Phys.*, 1974, **12**, 387.
15. Y. A. Chang, *Phys. Chem. Solidi*, 1967, **28**, 697.
16. J. C. Dugdale and D. K. C. MacDonald, *Phys. Rev.*, 1953, **89**, 832.
17. R. O. Davies and S. Parkes, *Phil. Mag. (GB)*, 1959, **4**, 341.
18. W. A. Basset, T. Takahari, H. K. Mao and J. S. Weaver, *J. Appl. Phys. (USA)*, 1968, **39**, 319.
19. J. H. Hildebrand, *Z. Phys. (German)*, 1931, **44**, 4618.
20. T. C. Waddington, *Adv. Inorg. Chem. Radiochem.*, 1959, **1**, 158.
21. F. D. Rossini, D. D. Wagman, W. H. Evans, S. Levino and I. Jaffe, "Selected values of Chemical Thermodynamic Properties Cire Natt Bur. St. and No. 500", US. Govt. Printing Office, Washington, DC, 1952.
22. K. P. Thakur, *Z. Phys. Chem.*, 1975d, **256**, 529.
23. B. Ghatak and J. Mandal, *J. Indian Chem. Soc.*, 2007, **84**, 820.
24. O. L. Anderson, *J. Phys. Chem. Solids*, 1966, 547.
25. Biswajit Ghatak and Jagdhar Mandal, *J. Indian Chem. Soc.* (communicated).