ANALYSIS OF POTENTIAL ENERGY DERIVATIVES BASED ON THE STACEY EQUATION OF STATE

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RECEIVED : 18 December, 2018

The derivatives of potential energy functions for some solids viz. Ne, Ar, Al, Cu, LiH and MgO have been determined using the Stacey reciprocal K-primed equation of state. The bulk modulus is related to the second order derivative of the potential energy function with respect to interatomic distance. The higher order derivatives of potential energy function have been determined in terms of pressure and derivatives of bulk modulus up to third order. It is found that the higher order derivatives of the potential energy function beyond second order related to the anharmonic behaviour of solids.

KEYWORDS : Potential energy functions, Pressure derivatives of bulk modulus, Higher order derivatives potential energy, Anharmonic behaviour.

INTRODUCTION

Equation of state (EOS) for a material can be obtained by taking the first derivative of potential energy function with respect to interatomic distance. Thus, we can write [1]

$$P = -\frac{d\emptyset}{dV} \qquad \ldots (1)$$

The bulk modulus K is then obtained using the relationship [2]

$$K = -V\frac{dP}{dV}$$
$$= V\frac{d^2\emptyset}{dV^2} \qquad \ldots (2)$$

When the interatomic distance r in a solid is changed from its equilibrium value r_0 at the atmospheric pressure $P = 0$, then the potential energy function can be written as

$$\phi(r) = \phi(r_0) + (r - r_0)\phi'(r_0) + \frac{(r - r_0)^2}{2}\phi(r_0) + \frac{(r - r_0)^3}{6}\phi'(r_0)$$
$$+ \frac{(r - r_0)^4}{24}\phi\text{iv}(r_0) + \frac{(r - r_0)^5}{120}\phi\text{v}(r_0) + \ldots\ldots \qquad \ldots (3)$$

where is the potential energy at $r = r_0$. The primes represent various order derivatives of with respect to r. The higher order derivatives beyond second order are related to the anharmonic behaviours of solids [3].

We determine the potential energy function with respect to interatomic distance up to fifth order in case of Ne, Ar, Al, Cu LiH, and MgO using the Stacey reciprocal K-primed equation of state [4-6]. The results for the pressure derivatives of bulk modulus reported recently [7] have been used in the present study.

METHOD OF ANALYSIS

The potential energy functions due to Rydberg [8] Mores [9] and Davydov [1] have been described in detail by Dharmendra [10-12]. Using the expressions given Stacey and Davis [5] for the pressure derivatives of bulk modulus. We drive the following equations (4), (5), (6) and (7).

$$\frac{r\Phi''}{\Phi'} = -\frac{3K}{P} + 2 \quad \ldots (4)$$

$$\frac{r^2\Phi'''}{\Phi'} = \frac{9K}{P}\left(K' - 1\right) + 2 \quad \ldots (5)$$

$$\frac{r^3\Phi iv}{\phi'} = -\frac{3K}{P}\left(9K'^2 + 9K'K'' - 9K' + 2\right) \quad \ldots (6)$$

$$\frac{r^4\,\Phi v}{\Phi'} = -\frac{3K}{P}\left(-27K'^3 - 108\,KK'K'' - 27K'^2K''' + 18KK'' + 18K'^2 + 3K' - 2\right) \ldots (7)$$

We calculate values of higher order derivatives of potential energy function Φ'', Φ''', Φ^{iv} and Φ^{v} by using equations (4) to (7). The results are given in Tables 1 to 4 for beyond solids viz. Ne, Ar, Al, Cu, LiH and MgO.

RESULTS AND CONCLUSIONS

The results has been found that the higher order derivatives of potential energy functions up to fifth order can be determine with the help of pressure derivatives of bulk modulus.The pressure derivatives of bulk modulus provides a direct method of investigation .The thermal and anharmoncity properties of material [5]. We have presented that results in the form of ratio of higher order derivatives of potential energy functions to the first order derivatives of potential energy function .The term beyond the second order derivative of potential functions have are directly related to the anharmonic behaviour of material. Using these derivatives of potential energy functions we can calculate properties such as GrÜniesian parameter and thermal expansivity of material. It should be mention that the ratio of higher order derivatives of potential energy function become are larger as compare to the lower order derivative of potential energy derivative viz. Potential energy functions. It has been found that the magnitude of the derivatives of potential energy functions or the ratios of derivatives potential energy functions decreases with increasing pressure. This reveals that an harmonic character of solids is suppressed at higher pressure in case of all the material under study.

ACKNOWLEGEMENT

The author is sincerely thankful to Dr. Jai Shanker, (Ex. Professor and head) department of physics, Dr. B.R. Ambedkar University, Agra for his valuable guidance and useful discussions. We are also thankful to Smt. Richa Singh for her computational help.

Table 1

Solids	(v/v_0)	P (GPa)	K (GPa)	ϕ''/ϕ'
Ne	0.9	0.996	13.2	-37.8
	0.8	3.26	26.8	-22.7
	0.7	8.62	56.8	-17.8
	0.6	22.3	130	-15.5
	0.5	62.4	343	-14.5
Ar	0.9	0.956	12.4	-36.9
	0.8	3.04	24.1	-21.8
	0.7	7.7	48.5	-16.9
	0.6	19	105	-14.6
	0.5	50.1	257	-13.4
Al	0.9	9.85	117	-33.6
	0.8	27.6	189	-18.5
	0.7	60.4	312	-13.5
	0.6	124	540	-11.1
	0.5	262	1012	-9.58
Cu	0.9	19.4	240	-35.1
	0.8	57.7	425	-20.1
	0.7	136	774	-15.1
	0.6	305	1497	-12.7
	0.5	763	3196	-10.6
LiH	0.9	4.95	55.5	-31.6
	0.8	12.8	79.3	-16.6
	0.7	25.7	115	-11.4
	0.6	47.7	174	-8.94
	0.5	88.1	276	-7.40
MgO	0.9	20.8	242	-32.9
	0.8	56.5	373	-17.8
	0.7	120	589	-12.7
	0.6	238	969	-10.2
	0.5	476	1707	-8.76

Table 2

Solids	(v/v_0)	*P* (GPa)	*K* (GPa))	*K*′	ϕ''/ϕ'
Ne	0.9	0.996	13.2	6.37	643
	0.8	3.26	26.8	5.79	356
	0.7	8.62	56.8	5.49	268
	0.6	22.3	130	5.34	230
	0.5	62.4	343	5.26	213
Ar	0.9	0.956	12.4	5.96	581
	0.8	3.04	24.1	5.41	317
	0.7	7.7	48.5	5.11	235
	0.6	19	105	4.95	199
	0.5	50.1	257	4.87	181
Al	0.9	9.85	117	4.26	351
	0.8	27.6	189	3.89	180
	0.7	60.4	312	3.65	125
	0.6	124	540	3.5	100
	0.5	262	1012	3.4	85
Cu	0.9	19.4	240	5.04	452
	0.8	57.7	425	4.64	243
	0.7	136	774	4.37	175
	0.6	305	1497	4.21	144
	0.5	763	3196	4.12	120
LiH	0.9	4.95	55.5	3.16	220
	0.8	12.8	79.3	2.91	109
	0.7	25.7	115	2.73	71
	0.6	47.7	174	2.6	55
	0.5	88.1	276	2.5	44
MgO	0.9	20.8	242	3.86	302
	0.8	56.5	373	3.54	153
	0.7	120	589	3.31	104
	0.6	238	969	3.16	81
	0.5	476	1707	3.06	69

Table 3

Solids	(v/v_0)	P (GPa)	K (GPa)	K'	KK''	$(\phi iv/\phi')10^2$
Ne	0.9	0.996	13.2	6.37	-9.6	-88.9
	0.8	3.26	26.8	5.79	-5.37	-50.1
	0.7	8.62	56.8	5.49	-3.64	-37.8
	0.6	22.3	130	5.34	-2.89	-32.3
	0.5	62.4	343	5.26	-2.51	-29.9
Ar	0.9	0.956	12.4	5.96	-8.64	-74.1
	0.8	3.04	24.1	5.41	-4.84	-41.2
	0.7	7.7	48.5	5.11	-3.21	-30.6
	0.6	19	105	4.95	-2.46	-25.8
	0.5	50.1	257	4.87	-2.11	-23.5
Al	0.9	9.85	117	4.26	-5.05	-29.1
	0.8	27.6	189	3.89	-2.72	-16.2
	0.7	60.4	312	3.65	-2.03	-11.0
	0.6	124	540	3.5	-1.49	-8.80
	0.5	262	1012	3.4	-1.17	-7.52
Cu	0.9	19.4	240	5.04	-6.34	-47.6
	0.8	57.7	425	4.64	-3.92	-26.2
	0.7	136	774	4.37	-2.61	-19.0
	0.6	305	1497	4.21	-1.94	-15.6
	0.5	763	3196	4.12	-1.6	-13.0
LiH	0.9	4.95	55.5	3.16	-2.99	-12.3
	0.8	12.8	79.3	2.91	-1.93	-6.44
	0.7	25.7	115	2.73	-1.32	-4.38
	0.6	47.7	174	2.6	-0.94	-3.39
	0.5	88.1	276	2.5	-0.69	-2.78
MgO	0.9	20.8	242	3.86	-4.23	-22.1
	0.8	56.5	373	3.54	-2.64	-11.7
	0.7	120	589	3.31	-1.73	-8.13
	0.6	238	969	3.16	-1.23	-6.40
	0.5	476	1707	3.06	-0.94	-5.41

Table 4

Solids	(v/v_0)	P (GPa)	K (GPa)	K'	KK''	K^2K'''	$(\phi v/\phi')10^4$
Ne	0.9	0.996	13.2	6.37	-9.6	141	14.3
	0.8	3.26	26.8	5.79	-5.37	64.8	7.67
	0.7	8.62	56.8	5.49	-3.64	39.3	5.69
	0.6	22.3	130	5.34	-2.89	28.8	4.80
	0.5	62.4	343	5.26	-2.51	24.7	4.45
Ar	0.9	0.956	12.4	5.96	-8.64	119	11.1
	0.8	3.04	24.1	5.41	-4.84	54.8	5.88
	0.7	7.7	48.5	5.11	-3.21	32.2	4.29
	0.6	19	105	4.95	-2.46	23	3.59
	0.5	50.1	257	4.87	-2.11	19	3.26
Al	0.9	9.85	117	4.26	-5.05	52.4	3.32
	0.8	27.6	189	3.89	-2.72	23.1	1.72
	0.7	60.4	312	3.65	-2.03	15.3	1.11
	0.6	124	540	3.5	-1.49	10.3	0.88
	0.5	262	1012	3.4	-1.17	7.57	0.74
Cu	0.9	19.4	240	5.04	-6.34	75.1	6.22
	0.8	57.7	425	4.64	-3.92	39.1	3.23
	0.7	136	774	4.37	-2.61	22.9	2.27
	0.6	305	1497	4.21	-1.94	15.8	1.86
	0.5	763	3196	4.12	-1.6	12.4	1.54
LiH	0.9	4.95	55.5	3.16	-2.99	23.6	1.13
	0.8	12.8	79.3	2.91	-1.93	12.8	0.52
	0.7	25.7	115	2.73	-1.32	7.68	0.34
	0.6	47.7	174	2.6	-0.94	4.89	0.25
	0.5	88.1	276	2.5	-0.69	3.33	0.21
MgO	0.9	20.8	242	3.86	-4.23	40.1	2.34
	0.8	56.5	373	3.54	-2.64	20.9	1.12
	0.7	120	589	3.31	-1.73	11.9	0.75
	0.6	238	969	3.16	-1.23	7.66	0.58
	0.5	476	1707	3.06	-0.94	5.57	0.49

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