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Pressure dependence of elastic constants for intermetallic compounds

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ABSTRACT: Elastic properties of solids are closely related to many fundamental properties such as EOS, thermal expansion, interatomic potentials etc. The relatively strong covalent bonding between the constituents of intermetallic compounds like LiBC, MgB_2 and TiB_2 gives high Bulk Modulus in the range 150-220 GPa at high melting point nearly 3000K. This behaviour makes these compounds very interesting for studies under high pressure and high temperature. In the present study, pressure-volume relationship at different temperatures for three intermetallic compounds is given. For the low compressions the increase in pressure is low but the rate of increase of pressure increases faster as we approach the high compression region. At higher temperature, the bulk modulus decreases and, therefore, the pressure required for producing same amount of compression becomes less and less.

Keywords: Intermetallic compounds, pressure, Bulk Modulus, Isotherm, parameter.

INTRODUCTION

The variations of thermoelastic properties of solids at high temperature can be understood by using adequate form of EOS and by studying the thermal emissivity, bulk modulus and other properties [1-3]. The pressure-volume relationship at constant temperature of the mineral gives isothermal compressibility. The Murnaghan's equation as well as the Birch Murnaghan equation needs to be modified if we have to predict the pressure-volume relationship at elevated temperatures. Such modifications should be introduced in order to incorporate the effect of thermal pressure.

In order to understand the thermoelastic behaviour of solids adequately under the effect of pressure and at high temperatures, we have to develop models for estimating the variations of Bulk Modulus [4]. The pressure dependence of elastic constants has attracted the attention of theoretical as well as experimental workers because of their requirement in geophysical and geochemical problems. It is desirable to investigate high derivative thermoelastic properties and Equation of State (EOS) at high pressure and high temperature. These properties can be determined with the help of an EOS having a fundamental basis.

MATERIAL AND METHODS

The general form of the strain in terms of volume ratio $\frac{V}{V_0}$ where V_0 is volume at P=0 is defined as [5]:

$$f = \frac{1}{n}\left(x^{-n/3} - 1\right) \qquad \text{-------------------(1)}$$

Where $x = \frac{V}{V_0}$ $and\ n = 2\ for\ Eulerian\ strain$

The reference state for Eulerian strain is deformed state.

Within the framework of strain theory developed by Stracey [6] free energy is expanded as:

$$H = H_0 + C_2 f^2 + C_3 f^3 \qquad \text{------------------ (2)}$$

Where; H_0 = free energy for reference state; C_2 *and* C_3 are coefficients in power series expansion; f is parameter as defined by equation 1.

The pressure-volume relationship along isotherms at different temperatures is obtained using Birch Murnaghan third order EOS [7& 8] which is derived from Eulerian strain theory and given as:

$$p = \frac{3}{2} K_0 \left(x^{-7/3} - x^{-5/3}\right) \left[1 + \frac{3}{4}(K_0' - 4)(x^{-2/3} - 1)\right] \quad \text{-------------(3)}$$

Where K_0, K_0' are the values of isothermal Bulk Modulus and its first pressure derivative $\frac{dK}{dP}$ $at\ P = 0$.

The values of Bulk Modulus $K_0(T)$ at different temperatures are obtained as:

$$K_0(T) = K_0(0) + A_1T - A_2T^2 + A_3T^3 \qquad \text{------------(4)}$$

Where $A_1 = 3.94\ X\ 10^{-3}$, $A_2 = 6.5241\ X\ 10^{-5}$ and $A_3 = 2.7048\ X\ 10^{-8}$ and

$K_0(0) = 170.3\ GPa\ for\ LiBC, 151\ GPa\ for\ MgB_2\ and\ 213\ GPa\ for\ TiB_2$

The change in K_0' with the temperature for different materials has been studied by Upadhyaya and Sharma[10]. It has been found that the rate of change of K_0' with temperature depends on the value of Bulk Modulus. Depending upon their method we have estimated:

$$\frac{dK_0'}{dT} = 0.3\ X\ 10^{-3}\ K^{-1}\ for\ LiBC\ and\ MgB_2$$

&

$$\frac{dK_0'}{dT} = 0.2\ X\ 10^{-3}\ K^{-1}\ for\ TiB_2$$

The input parameter K_0 and K_0' are thus obtained for LiBC, MgB_2 and TiB_2 are reported in Table 1.

Bina and Helffrich [9] have formulated a third order Eulerian strain equation of state for elastic constants as:

$$C_{ij} = C_{ij}^0\ (1+f)^{5/2} \left[1 - f\left\{5 - 3\left(\frac{dC_{ij}}{dP}\right)_0 \left(\frac{K_0}{C_{ij}}\right)\right\}\right] \quad \text{--------------(5)}$$

Where

$$f = \frac{1}{2}\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right] \qquad \text{--------------(6)}$$

It has been assumed that the relative changes in elastic constants and bulk modulus are i.e.

$$\frac{1}{C_{ij}^0}\left(\frac{dC_{ij}}{dP}\right)_0 = \frac{1}{K_0}\left(\frac{dK}{dP}\right)_0 \qquad \text{---------------(7)}$$

Using eq. (5) and (7), we get:

$$\frac{C\ ij}{C_{ij}^0} = (1+f)^{5/2}\left\{1 - f\ \left[5 - 3\left(\frac{dK}{dP}\right)_0\right]\right\} \qquad \text{---------------(8)}$$

Here $\quad C_{ij}\ is\ C_{ij}\ (T,P) and\ C_{ij}^0 = C_{ij}\ (T,0)$

Equation [8] can be used to predict pressure dependence of elastic constants at a given temperature for materials provided values of K_0' is known at that temperature

Upadhyay and Sharma [10] calculated pressure-volume relationship at different temperatures using eq. (3) for three intermetallic compounds viz. LiBc, MgB_2 and TiB_2. The input data of $K_{0,}$ K_0' used in the calculations are given in Table 1.

At P=0 for $V=V_0$, we can determine the value of elastic constants at different temperatures using the relation [11].

$$C_{ij}(T) = C_{ij}(0) + A_1T - A_2T^2 + A_3T^3 \qquad \text{---------------(9)}$$

RESULTS AND DISCUSSION

The pressure-volume results of LiBc, MgB_2 and TiB_2 are reported in Table 2, Table 3 and Table 4 respectively.

Values of volume ratio represented by $\frac{V}{V_0}$ are infact $\frac{V\ (T,P)}{V\ (T,0)}$ i.e. Isothermal compression.

At each temperature T, we have $\frac{V\ (T,P)}{V\ (T,0)} = 1\ at\ P\ = 0$

As the volume is decreased, pressure increases.

In the starting i.e. for low compressions ($\frac{V}{V_0}\ from\ 1\ to\ 0.9$) the increase in pressure is slow but the rate of increase of pressure increases and becomes faster and faster as we approach the high compression region. This explains why the pressure-volume relationships are nonlinear. At higher temperature, the bulk modulus decreases and therefore the pressure required for producing the same amount of compression at higher temperature becomes less and less. Values of elastic constants thus determined at elevated temperatures T= 0K, 300K, 600K and 900K have been used in equation (8) to find elastic constants at elevated pressures along different isothermals.

The results of $C_{ij}(T,P)$ for LiBC, MgB_2 and TiB_2 are reported in table 2, table 3 and table 4 respectively.

Table 1: Input values of K_0(GPa) and K_0' for LiBC, MgB_2 & TiB_2

T(K)	LiBC		MgB_2		TiB_2	
	K_0 (GPa)	K_0'	K_0 (GPa)	K_0'	K_0 (GPa)	K_0'
0	170.3	3.76	151	4.0	213	2.10
300	166.3	3.85	147	4.09	200	2.16
600	155	3.94	135.7	4.18	197.7	2.22
900	140.3	4.03	121.4	4.27	183.4	2.28

Table 2: Values of elastic constants at different pressures and temperatures for LiBC.

V/V_0	0 K				300 K				600 K				900 K			
	P (GPa)	C_{11}	C_{12}	C_{44}	P (GPa)	C_{11}	C_{12}	C_{44}	P (GPa)	C_{11}	C_{12}	C_{44}	P (GPa)	C_{11}	C_{12}	C_{44}
1	0	638	117	123	0	634	113	119	0	622	102	108	0	608	87.4	93.4
0.95	9.60	770	141	148	9.42	768	137	144	8.80	757	124	131	7.98	743	107	114
0.90	21.8	933	171	180	21.5	935	167	175	20.1	925	152	161	18.3	911	131	140
0.85	37.5	1136	208	219	36.9	1142	203	214	34.7	1132	186	197	31.7	1119	161	172
0.80	57.6	1391	255	268	56.9	1401	250	263	53.7	1394	229	242	49.2	1382	199	213
0.75	83.7	1713	314	330	83.2	1732	309	325	78.6	1727	283	300	72.2	1716	247	264
0.70	118	2129	390	410	118	2157	384	405	112	2157	354	374	103	2148	309	330
0.65	164	2674	490	515	164	2715	484	510	156	2721	446	472	145	2716	390	417
0.60	224	3397	623	655	226	3458	616	217	217	3472	569	603	202	3472	499	533

Table 3: Values of elastic constants at different pressures and temperatures for MgB_2.

V/V_0	0 K				300 K				600 K				900 K			
	P (GPa)	C_{11}	C_{12}	C_{44}	P (GPa)	C_{11}	C_{12}	C_{44}	P (GPa)	C_{11}	C_{12}	C_{44}	P (GPa)	C_{11}	C_{12}	C_{44}
1	0	462	67.0	80.0	0	458	63.0	76.0	0	447	51.7	64.7	0	432	37.4	50.4
0.95	8.58	562	81.5	97.3	8.38	559	76.9	92.8	7.75	548	63.4	79.3	6.95	532	46.0	62.0
0.90	19.7	688	99.8	119	19.2	687	94.6	114	17.8	676	78.2	97.8	16.0	658	57.0	76.8
0.85	34.0	846	123	147	33.4	848	117	141	31.0	837	96.8	121	27.9	817	70.8	95.3
0.80	52.7	1044	151	181	51.9	1050	144	174	48.4	1038	120	150	43.7	1017	88.0	119
0.75	77.3	1291	187	224	76.4	1300	179	216	71.5	1290	149	187	64.8	1266	110	148
0.70	110	1621	235	281	109	1637	225	272	103	1627	188	235	93.4	1601	139	187
0.65	154	2045	297	354	154	2069	285	343	145	2061	238	298	133	2031	176	237
0.60	215	2605	378	451	215	2640	363	438	204	2634	305	381	187	2601	225	303

Table 4: Values of elastic constants at different pressures and temperatures for TiB_2.

V/V_0	0 K				300 K				600 K				900 K			
	P (GPa)	C_{11}	C_{12}	C_{44}	P (GPa)	C_{11}	C_{12}	C_{44}	P (GPa)	C_{11}	C_{12}	C_{44}	P (GPa)	C_{11}	C_{12}	C_{44}
1	0	660	48.0	260	0	656	44.0	256	0	645	32.7	245	0	630	18.4	230
0.95	11.5	733	53.3	289	11.3	731	49.0	285	10.7	720	36.5	274	9.96	706	20.6	258
0.90	24.9	822	59.8	324	24.5	822	55.1	321	23.2	813	41.2	309	21.6	799	23.3	292
0.85	40.1	928	67.5	366	39.6	932	62.5	364	37.7	324	46.8	351	35.2	912	26.6	333
0.80	57.4	1055	76.8	416	56.8	1063	71.3	415	54.2	1058	53.7	402	50.8	1047	30.6	382
0.75	76.2	1208	87.8	476	75.8	1220	81.8	476	72.7	1219	61.8	463	68.3	1210	35.3	442
0.70	96.0	1403	102	553	96.0	1423	95.4	555	92.6	1427	72.4	542	87.5	1421	41.5	519
0.65	115	1643	119	647	116	1672	112	653	112	1684	85.4	640	107	1684	49.2	615
0.60	128	1946	142	767	131	1990	133	776	129	2011	102	764	125	2018	58.9	737

CONCLUSION

It is found from the results that the elastic constants increase substantially with the increase in pressure along each isotherm at 0K, 300K, 600K and 900K. At P= 0, the elastic constants decrease with the increase in temperature. At higher compressions the change in elastic constants becomes small.

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