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Temperature dependence of Elastic Constants and Bulk Modulus of metals

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ABSTRACT: The temperature dependence of bulk modules was given by Q. Liu & Q. He[13] using fundamental thermodynamic relations. The assumption in this theory was that volume thermal expansion coefficient is quadratic function of temperature. The new expressions and formulations were also derived by Tallon[14]. In the present study temperature of elastic constants is based on the combination of above mentioned formulations. A method to estimate the temperature dependence of bulk modules is developed with the approximation that coefficient of volume thermal expansion depends linearly on temperature. This approximation is valid only for small expansions in low temperature range.

Keywords: Elastic Constant, Temperature Dependence and Bulk Modulus.

INTRODUCTION

The temperature dependence of elastic constants has attracted the attention of theoretical as well as experimental workers [1-6] because of their requirement in geophysical and geochemical problems. For the temperature dependence of elastic properties, rigid ion mode is based on Monte Carlo and Lattice Dynamics studies. Singh et.al. [7&8] developed a three body potential model for the temperature variation of elastic constants. A simple theoretical method has been suggested by Lazarus and Spetzler et.al.[9]. Singh et.al.[10] suggested a simple method for determination of effect of temperature on elastic modulii. The expressions for second order elastic constants (SOEC) have been reported by Wellace[11] to study cubic crystals under isotropic pressure[12].

MATERIAL AND METHODS

The SOEC at temperature T and T_0 are given as-

$$C_{11} = C_{11}^0 - P_{phonon} \text{ ---------(1)}$$

$$C_{12} = C_{12}^0 + P_{phonon} \text{ ----------(2)}$$

$$C_{44} = C_{44}^0 - P_{phonon} \text{ ----------(3)}$$

Where C_{ij} represent the SOEC at temperature T and C_{ij}^0 are their values at T=T_0.
Thermal Pressure may be evaluated in the traditional way [2].

$$\left(\frac{\partial P}{\partial T}\right)_V = \left(\frac{\partial P_{Th}}{\partial T}\right)_V$$

$$= \propto_0 K_0 \qquad \text{[Where v is the volume]}$$

$$P_{Th} = \int_{T_0}^{T} \propto_0 K_0 \, dT$$

or $$P_{Th} = \propto_0 K_0 (T - T_0) \text{---------(4)}$$

Where $\propto_0$ and K_0 are coefficients of volume thermal expansion and bulk modulus respectively and 0 refers to their values at$T = T_0$.
In the present study the temperature is considered higher than room temperature. For most of the solids considered in the present study, the Debye temperature is close to the room temperature. The temperature dependence of C_{ij} is given as

$$\frac{C_{ij}}{C_{ij}^0} = 1 \pm \frac{\propto_0 K_0 (T-T_0)}{C_{ij}} \quad \text{----------(5)}$$

Q. Liu and Q. He [13] developed a new expression for the temperature dependence of bulk modulus by using fundamental thermodynamic relations simultaneously assuming that the volume thermal expansion is a quadratic function of temperature. By combining the new expression with the formulation derived from Tallon's model [14], we calculated the temperature dependence of elastic constants. The Anderson Gruneisen parameter is defined as

$$\delta_T = -\frac{1}{\propto K_T}\left(\frac{\partial K_T}{\partial T}\right)_\rho \quad \text{----------(6)}$$

Where $\propto$ and K_T are coefficient of volume thermal expansion and isothermal bulk modulus respectively.

$$\propto = \frac{1}{V}\left(\frac{\partial v}{\partial T}\right)_P \quad \text{----------(7)}$$

and

$$K_T = \frac{1}{V}\left(\frac{\partial P}{\partial V}\right)_T \quad \text{----------(8)}$$

A method to estimate the temperature dependence of bulk modulus has been developed with the approximation that $\propto$ depends linearly on temperature. This approximation is valid for low temperature range.

$$\propto = \propto_0 + \propto_0' (T - T_0) + \frac{\propto_0''}{2}(T - T_0)^2 \text{ -------(9)}$$

Where $\propto_0' \; and \; \propto_0''$ are the first and second order derivative of $\propto$ at initial temperature T=T_0.
If the product $\propto K_T$ is assumed to be constant then from eq. (6):
We get

$$\delta_T = \frac{1}{\propto^2}\left(\frac{\partial \propto}{\partial T}\right)_\rho \quad \text{----------(10)}$$

$$\propto_0' = \left(\frac{\partial \propto}{\partial T}\right)_P$$

$$= \delta_{T_0} \propto_0^2$$

and

$$\propto_0'' = \left(\frac{\partial^2 \propto}{\partial T^2}\right)_P$$

$$= 2\delta_{T_0}^2 \propto^3$$

So eq. (9) can be written as:

$$\propto = \propto_0 + \delta_{T_0} \propto_0^2 (T - T_0) + \delta_{T_0}^2 \propto_0^3 (T - T_0)^2 \quad \text{----------(11)}$$

Using eq. (6) and (11), we get:

$$\frac{dK_T}{K_T} = -\delta_{T_0}\left[\propto_0 + \delta_{T_0} \propto_0^2 (T - T_0) + \delta_{T_0}^2 \propto_0^3 (T - T_0)^2\right] dT \quad \text{----------(12)}$$

Integrating eq. (12):

$$\frac{K_T}{K_{T_0}} = \exp[-\delta_{T_0} \propto_0 (T - T_0)\{1 + \frac{\delta_{T_0} \propto_0 (T-T_0)}{2} + \frac{\delta_{T_0}^2 \propto_0^2 T - T_0)^2}{3}\}] \text{----------(13)}$$

Grover et.al. [15] used a non standard definition of δ_T and recalled it the parameter g as:

$$g = -\frac{V_0}{K_T}\left(\frac{\partial K_T}{\partial v}\right)_\rho$$

The generalized form of this equation is:

$$g_m = -\frac{V_0}{M}\left(\frac{\partial M}{\partial V}\right)_P \quad \text{----------(14)}$$

Where M represents any of elastic modulii such as $C_{11}, C_{12}, C_{44}, \frac{C_{11}-C_{12}}{2}$ or K_T.

Tallon [14] expressed this equation as:

$$\frac{M}{M_0} = -\exp[g_m(\frac{v}{v_0}-1)] \quad \text{----------(15)}$$

This equation may be used to determine the temperature dependence of elastic constants.

Following the method of generalization eq. (13) can be expressed as:

$$\frac{M}{M_0} = \exp[-\delta_{M_0} \propto_0 (T-T_0)\{1 + \frac{\delta_{M_0}\propto_0(T-T_0)}{2} + \frac{\delta_{M_0}^2 \propto_0^2 T-T_0)^2}{3}\}] \text{---------(16)}$$

Here δ_{M_0} should vary according to the elastic modulii selected.

The relevant expression for elastic constants may be written collectively as:

$$\frac{C_{ij}}{C_{ij_0}} = \exp[-\delta_{ij_0} \propto_0 (T-T_0)\{1 + \frac{\delta_{ij}\propto_0(T-T_0)}{2} + \frac{\delta_{ij_0}^2 \propto_0^2 T-T_0)^2}{3}\}] \text{----------(17)}$$

When δ_{ij} is given by eq. (6) as defined by Kumar and Bedi [5].

In every pseudo formalism, either local or non local approach has been used for the calculation of metallic properties. Baria and Janib [16] proposed a local form of a pseudo potential.

In pseudo formalism, it is necessary that the potential parameter is determined properly. We have calculated the potential parameter from the zero pressure condition. The advantage of this method is that potential does not bear any constraint due to a fitting procedure with the experimentally observed physical properly. Hartee's static dielectric function along with the exchange and correction effects of Taylor's[17] screening function is used in the calculations. The value of binding energy at zero pressure condition is obtained using the formulation of Antonov et.al.[18].

$$E = E_i + E_s^{(0)} + E_s^{(1)} + E_s^{(2)} + \emptyset_{sr}$$

The last term in the above expression is Born-Mayer term and taken from Antonov et.al. [18].

RESULTS AND DISCUSSION

The calculated values of Binding Energy are shown in Table-1 and are compared with experimental findings [19] and other theoretical results. The present findings show excellent agreement with experimental values for Cu, Au and Ni, while it shows derivation for Ag, Pt and Rh. The present findings are better than the theoretical results of Pandya et.al. [20] and are comparable to the findings of Singh et.al. [21].

The experimental [22] and other theoretical values [21] of elastic constants C_{11}, C_{12}, C_{44} and Bulk Modulus along with the present findings are displaced in Table-2 at room temperature. Our present findings of elastic constants C_{11}, C_{12}, C_{44} and Bulk Modulus K for Cu, Au, Pt and Rh are very close to experimental findings. The temperature variations of elastic constants C_{11}, C_{12}, C_{44} and Bulk Modulus K are displaced in Table-3 and are compared with results Cagin et.al. [22] at various temperatures.

Table 1: Binding Energy in ryd./ele. at zero pressure condition

METAL			Cu	Ag	Au	Ni	Pt	Ph
R_C			1.107281	1.562870	1.638134	1.02570	1.401676	1.289722
VALENCE			1.5	1.5	2.0	1.5	1.5	1.5
BINDING	PRESENT		1.37871	1.16596	1.91339	1.42796	1.23039	1.28164
ENERGY	EXP [19]		1.3376	1.3075	2.0498	1.3612	1.5940	1.4273
IN RYD.	OTHERS	[20]	0.8348	0.7998	0.8499	2.1588	1.9939	-
		[21]	1.219	1.172	2.160	1.267	1.282	-
			1.244	1.208	2.222	1.282	1.311	-

Table 2: Elastic Constants C_{11}, C_{12}, C_{44} and Bulk Modulus K (in gpa) at room temperature.

Metals	C_{11}			C_{12}			C_{44}			K		
	Present	Expt. [22]	Others [18,21]	Present	Expt. [22]	Others [18,21]	Present	Expt. [22]	Others [18,21]	Present	Expt. [22]	Others [18,21]
Cu	174.71	168.39	153.06	128.72	121.42	119.45	64.49	75.39	49.35	144.05	137.07	130.65
			136.10			119.80			66.50			125.30
			153.50			123.40			77.30			133.40
Ag	108.41	123.99	126.95	88.97	93.67	88.49	58.82	46.12	50.50	95.45	103.77	101.31
			88.20			99.10			44.20			82.00
			112.20			96.90			50.90			102.00
Au	185.90	192.34	158.24	162.21	163.14	131.56	38.57	41.95	34.62	170.11	172.87	140.45
			150.00			128.60			70.30			135.70
			138.00			88.40			58.20			104.90
Ni.	233.10	250.80	213.76	158.01	150.00	166.50	121.94	123.50	69.77	183.04	183.60	182.30
			243.80			164.00			96.70			198.00
			175.50			159.40			116.3			164.70
Pt	323.74	346.70	289.63	245.87	250.87	239.55	72.31	76.50	65.07	271.83	282.70	256.24
			321.00			244.00			111.00			270.00
			231.00			177.80			125.50			195.50
Rh	393.92	412.60	322.30	202.42	193.50	223.02	189.39	184.10	131.95	266.25	266.53	256.11

Table 3: Elastic Constants C_{11}, C_{12}, C_{44} and K (in gpa) at various temperatures

Metals	Temp in K	C_{11}		C_{12}		C_{44}		K	
		Present	Others[22]	Present	Others[22]	Present	Others[22]	Present	Others[22]
Cu	300	174.71	153.06	128.72	119.45	64.49	49.35	144.05	130.65
	500	166.80	140.87	122.32	112.78	61.81	43.46	137.14	122.14
	750	156.45	126.46	113.97	104.43	57.74	36.37	128.13	111.77
	1000	144.82	109.09	104.62	94.40	53.15	27.92	118.02	99.30
Ag	300	108.41	126.95	88.97	88.49	58.82	50.50	95.45	101.31
	500	100.37	117.46	82.70	83.45	54.84	45.50	88.59	94.79
	750	90.41	104.16	74.90	76.79	49.86	37.75	80.7	85.91
	1000	80.20	91.88	66.86	70.59	44.69	31.54	71.31	77.69
Au	300	185.90	158.24	162.21	131.56	38.57	34.92	170.11	140.45
	500	175.96	141.74	153.35	118.92	34.64	30.08	160.88	126.52
	750	162.52	123.92	141.38	107.42	39.30	24.10	148.43	112.92
	1000	146.49	95.43	127.14	84.78	32.87	16.78	133.59	88.33
Ni	300	233.10	213.76	158.01	166.57	121.94	69.77	183.04	182.30
	500	223.95	201.70	150.46	159.48	117.57	63.56	174.95	173.55
	750	212.32	186.05	140.59	150.34	111.98	55.94	164.50	162.24
	1000	200.13	169.14	132.19	141.08	106.09	48.29	154.83	150.43
Pt	300	323.74	289.93	245.87	239.55	72.31	65.07	271.83	256.24
	500	307.22	272.67	233.55	227.11	64.92	59.67	258.10	242.29
	700	290.78	256.12	221.28	214.38	60.67	54.15	244.45	228.30

	750	286.56	251.09	218.14	211.05	55.03	52.90	240.95	224.34
	900	274.00	233.28	208.77	196.58	51.23	49.08	230.52	208.81
	1000	265.56	227.47	202.48	193.46	49.28	45.50	223.50	204.80
	1100	256.76	219.39	195.94	188.60	45.33	44.12	216.22	198.89
	1300	238.96	200.63	182.64	174.16	44.47	38.78	201.41	183.98
	1500	219.44	177.28	168.07	155.50	40.87	31.94	185.19	162.76
Rh	300	393.92	322.30	202.42	223.02	189.39	131.95	266.25	256.11
	500	378.69	312.03	191.01	216.89	182.53	124.72	253.57	248.60
	700	363.66	298.92	179.74	210.23	175.74	117.44	241.04	239.79
	750	359.82	265.14	176.87	207.72	174.00	116.27	237.85	236.86
	900	348.35	286.44	168.27	203.55	168.81	110.80	228.29	231.17
	1000	340.88	279.36	162.66	199.07	165.43	108.16	222.06	225.83
	1100	333.36	274.83	157.02	197.32	162.02	104.02	215.80	223.15
	1300	318.04	263.48	145.53	191.06	155.06	97.36	203.03	215.20
	1500	302.94	249.59	134.20	184.18	148.18	91.29	190.44	206.36

CONCLUSION

The present findings of elastic constants and Bulk Modulus for Cu, Au and Rh are better than Cagin et.al.[22] while for Ni and Pt it is excellent better and a little poor for Ag at room temperature. It is also better in comparison to theoretical values of Pandya et.al. [20] and Singh et.al. [21].

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