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Temperature dependent anharmonic properties of MgO, MgS and MgSe

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ABSTRACT

Data on elastic constants and associated properties at high temperature (100-1000K) for MgO, MgSe and MgS crystals are presented and discussed starting from primary physical parameters viz. nearest neighbour distance and hardness parameter assuming long- and short- range potentials. When the values of the higher order elastic constants are known for a crystal, many of the anharmonic properties of the crystal can be treated within the limit of the continuum approximation in a quantitative manner. If the values of second order elastic constants and density at a particular temperature are known for any substance, one may obtain ultrasonic velocities for longitudinal and shear waves which give an important information about its internal structure, inherent and anharmonic properties. Though compendiums of elastic constant data for numerous compounds exist, they are restricted to temperatures at or near room temperature. Current problems in material science often require values of elastic constants at elevated temperatures. The compounds of magnesium have attracted a lot of interest due to their complex physical and chemical characteristics. In past years, the physical properties of these substances have been studied. However, none of the work reported in the literature so far is centered on the study of temperature variation of anharmonic properties. Therefore, in this study, higher order elastic constants and related properties are computed upto 1000K for MgO, MgS and MgSe. The first order pressure derivatives of second and third order elastic constants, the second order pressure derivatives of second order elastic constants and partial contractions are also evaluated at different temperatures. The results thus obtained are compared with other available data and found in well agreement with present values.

INTRODUCTION

In last and present decade considerable interest has been taken in investigation of ultrasonic properties of materials [1-5]. Some investigators [2-5] have tried to obtain the second, hird and fourth order elastic constants (SOECs, TOECs and FOECs) for divalent crystals assuming that the elastic constants are linear function of temperature. The present theory deals with higher order elastic constants and physical properties of divalent crystals having face centered cubic crystal symmetry. In present investigation, some efforts have been made for obtaining the SOECs, TOECs and FOECs, the first order pressure derivatives (FOPDs) of the SOECs and TOECs, the second order pressure derivatives (SOPDs) of the SOECs and partial contractions of divalent crystals (MgO, MgSe and MgS) having face centered cubic crystal structure starting from nearest neighbour distance(r) and hardness parameter (q) utilizing the Coulomb and Börn-Mayer [15] potentials. The study is performed for the temperature range 100-1000K.

When the values of the higher order elastic constants are known for a crystal, many of the anharmonic properties of the crystal can be treated within the limit of the continuum approximation in a quantitative manner. If the values of second order elastic constants and density at a particular temperature are known for any substance, one may obtain ultrasonic velocities and attenuation for longitudinal and shear waves which give an important information about its internal structure, inherent and anharmonic properties.

FORMULATION

The elastic energy density for a crystal of a cubic symmetry can be expanded up to quartic terms as shown below [1,5]:

$$U_0 = U_2 + U_3 + U_4$$

$$= [1/2!]C_{ijkl}x_{ij}x_{kl} + [1/3!]C_{ijklmn}x_{ij}x_{kl}x_{mn} + [1/4!]C_{ijklmnpq}x_{ij}x_{kl}x_{mn}x_{pq} \quad (1)$$

Where C_{ijkl}, C_{ijklmn} and $C_{ijklmnpq}$ are the SOECs, TOECs and FOECs in tensorial form; x_{ij} are the Lagrangian strain components; C_{IJ}, C_{IJK} and C_{IJKL} are the SOECs, TOECs and FOECs in Brügger's definition and Voigt notations.The SOECs, TOECs and FOECs are as given below :

$$C_{ijkl} = C_{IJ} = (\partial^2 U/\partial x_{ij}\,\partial x_{kl})_{x=0}$$

$$C_{ijklmn} = C_{IJK} = (\partial^3 U/\partial x_{ij}\,\partial x_{mn}\,\partial x_{kl})_{x=0}$$

and $$C_{ijklmnpq}=C_{IJKL}=(\partial^4 U/\partial x_{ij}\,\partial x_{kl}\,\partial x_{mn}\,\partial x_{pq})_{x=0} \quad (2)$$

An elastic constant consists of two parts as follows

$$C_{IJ} = C^0_{IJ} + C_{IJ}^{vib};$$

$$C_{IJK} = C^0_{IJK} + C_{IJK}^{vib};$$

and $$C_{IJKL} = C^0_{IJKL} + C_{IJKL}^{vib} \quad (3)$$

The first part is the strain derivative of the internal energy U_o and is known as "static" elastic constant and the second part is the strain derivative of the vibrational free energy U^{vib} and is called "Vibrational" elastic constant. The superscript ""0"" has been introduced to emphasize that the static elastic constants correspond to 0K. By adding the vibrational elastic constants to the static elastic constants, one may get SOECs and TOECs at any temperature for FCC crystals. The general expressions for these properties have been reported in [1,5] and therefore are not repeated in this paper.

EVALUATION

The brief formulation is given in previous Section. Different expressions [1,5,6] for higher order elastic constants and pressure derivatives have been used for calculations.The second, third and fourth order elastic constants for MgO, MgSe and MgS are evaluated at room temperatures utilizing the concepts of the nearest neighbour distance and hardness parameter. Adding vibrational contribution to SOECs, TOECs and FOECs at 0K, the second, third and fourth order elastic constants for MgO, MgSe and MgS are evaluated at room temperature. The evaluation for the first and second order pressure derivatives of SOECs and the FOPDs of TOECs for MgO, MgSe and MgS is made using room temperature data. Results at room temperature are shown in Tables 1-3 alongwith other theoretical data for comparision.The temperature variations of above anharmonic properties for 100K-1000K are presented in Figures 1-8.

RESULTS AND DISCUSSION

Though compendiums of elastic constant data for numerous compounds exist, they are restricted to temperatures at or near room temperature. Current problems in material science often require values of elastic constants at elevated temperatures. The compounds of magnesium have attracted a lot of interest due to their complex physical and chemical characteristics. In past years, the physical properties of these substances have been studied. However, none of the work reported in the literature so far is centered on the study of temperature variation of anharmonic properties. Therefore, in this study, higher order elastic constants and related properties are computed upto 1000K for MgO, MgS and MgSe.

The SOECs and TOECs in 10^{10} Newton/meter^2 at room temperature of MgO, MgSe and MgS are shown in Table 1. The theoretical [7,8,9] and experimental [9] values of the elastic constants evaluated by other investigators are also given. It is obvious from Table 1that there are three independent SOECs at room temperature. One may state that all the SOECs are positive in nature. The temperature dependence of SOECs is shown in Figure 1. From Table 1, it is clear that there are six TOECs at room temperature. The experimental and theoretical values are also in agreement with present results. Figure 2 shows the variation of third order elastic constants with temperature.

The FOECs and partial contractions at room temperature are shown in Figure 3. There are eleven FOECs for MgO, MgSe and MgS at 300K. For all crystals, C_{1112}, C_{1122}, C_{1123}, C_{1144}, C_{1255}, C_{1456} and C_{4455} are negative in nature and C_{1155}, C_{1266} and C_{4444} are positive. Figure 4 represents the tempertaur variation of partial contraction Y_{11} for these compounds.

The FOPDs and SOPDs of the second and third order elastic constants are shown in Table 2 and in Figs 5, 6 and 7. One may state that the first order pressure derivative of C_{11} is negative and others are positive in nature for all crystals. The experimental values [10-11] of the FOPDs of SOECs for MgO are in agreement with present results. For most of the crystals, SOPDs of SOECs are negative in nature. The magnitude and the order of theoretical values of other workers [8] for SOPDs of SOECs are in agreement with present results. The FOPDs of TOECs are presented in Table 3 and in Figure 8 for MgO, MgSe and MgS. The FOPDs of C_{144} are negative in nature while others are positive in present study.

The cases discussed in present study are in overall good agreement with theoretical and experimental results, which shows the validity of present theory. The data obtained in present investigation will be helpful to those workers who are engaged in such studies. The new data may provide a further chance to improve the theoretical models developed recently for the interpretation of the behavior of elastic constants in higher temperature region.

Acknowledgement

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Table 1. SOECs and TOECs in 10^{10} N/m^2 at room Temperature.

Comp.	C_{11}	C_{12}	C_{44}	C_{111}	C_{112}	C_{123}	C_{144}	C_{166}	C_{456}	Ref.
MgO	27.03	11.06	10.98	-371.50	-85.59	30.45	31.83	-88.48	31.08	
				-240.48	-86.20	30.06	30.84	-58.20	30.79	[7]
	29.40	9.24	15.58	-328.00	-31.80	24.20	31.80	-67.40	35.60	[8]
				-489.50	-95.00	-6.90	11.30	-65.90	14.70	[9]
MgSe	15.88	7.998	7.781	-246.91	-31.07	11.16	12.10	-31.77	12.03	
				-238.26	-28.25	10.82	10.90	-28.40	10.88	[7]
MgS	17.38	10.44	10.67	-258.95	-42.72	15.22	16.14	-43.42	16.05	
				-247.20	-34.78	13.10	13.18	-34.93	13.14	[7]

Table 2. The FOPDs and SOPDs of the SOECs in 10^{-11} N/^{2}.

Comp.	$\frac{dC_{11}}{dP}$	$\frac{dC_{12}}{dP}$	$\frac{dC_{44}}{dP}$	$\frac{dS}{dP}$	$\frac{dK}{dP}$	$\frac{d^2C_{11}}{dP^2}$	$\frac{d^2C_{12}}{dP^2}$	$\frac{d^2C_{44}}{dP^2}$	Ref.
MgO	-4.83	2.32	1.08	0.88	3.66	-0.89	-0.84	-0.16	
			4.20a	2.47b	3.27b	-0.69b	-0.15b	-0.18b	[7a,8b]
			1.12	3.67	4.29				[10]
			1.2						[11]
MgSe	-8.14	1.88	0.36	2.89	4.28	0.48	-0.48	0.02	
MgS	-7.29	1.99	0.53	2.39	4.11	-0.13	-0.68	-0.06	

Table 3. The FOPDs of the TOECs in 10^{-11} N/m^2.

Comp.	$\frac{dC_{111}}{dP}$	$\frac{dC_{112}}{dP}$	$\frac{dC_{123}}{dP}$	$\frac{dC_{144}}{dP}$	$\frac{dC_{166}}{dP}$	$\frac{dC_{456}}{dP}$	Ref.
MgO	249.7	276.1	288.5	-1.35	93.07	3.12	
	44.9	140.0	229.0	-1.73	25.0	4.43	[8]
MgSe	4.09	79.12	88.74	-1.25	27.46	2.51	
MgS	67.41	128.8	139.2	-1.27	44.01	2.64	

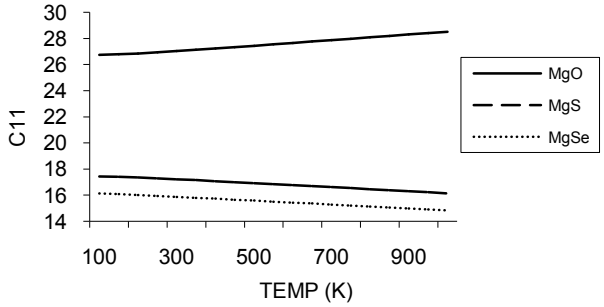

Figure 1. C_{11} (in 10^{10} N/m^2) for Magnesium Compounds.

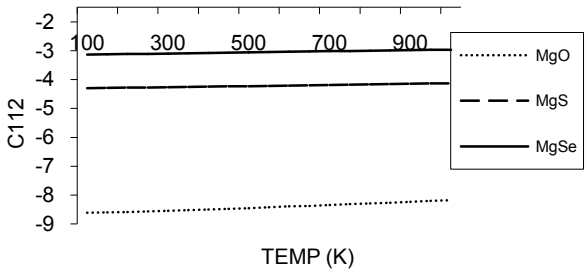

Figure 2. Temperature variation of TOECs (in 10^{11} N/m^2).

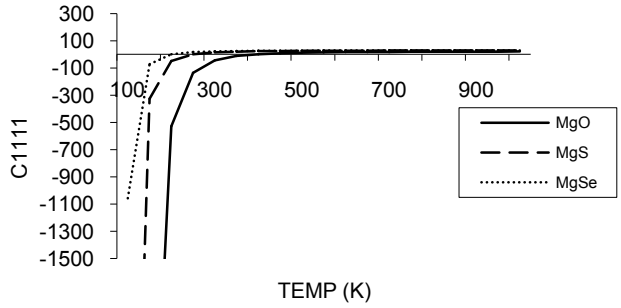

Figure 3. Temperature variation of FOECs (in 10^{12} N/m^2).

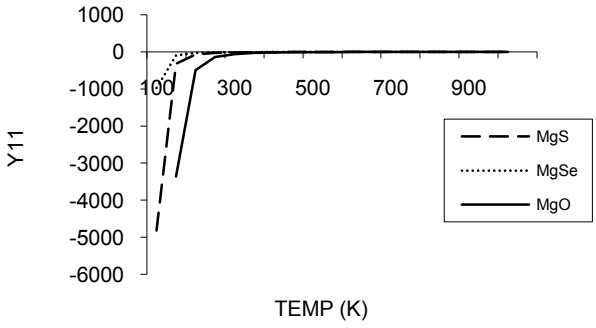

Figure 4. Variation of partial contraction (in 10^{14}).

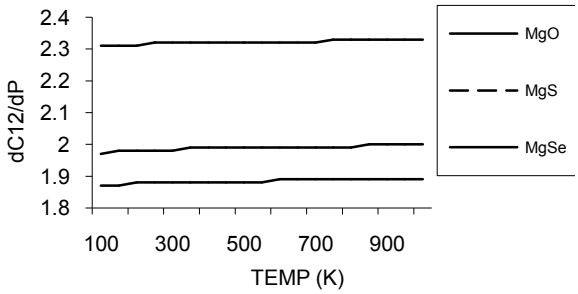

Figure 5. Temperature variation of FOPD of C_{12}.

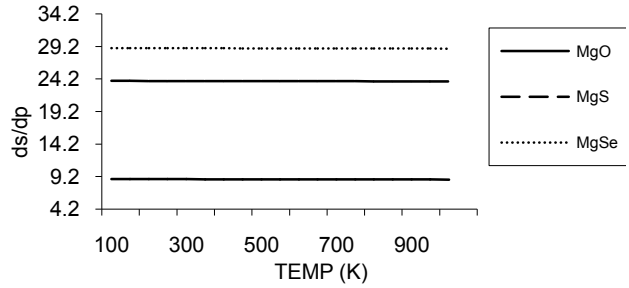

Figure 6. Temperature variation of ds/dp (X10^{-1}).

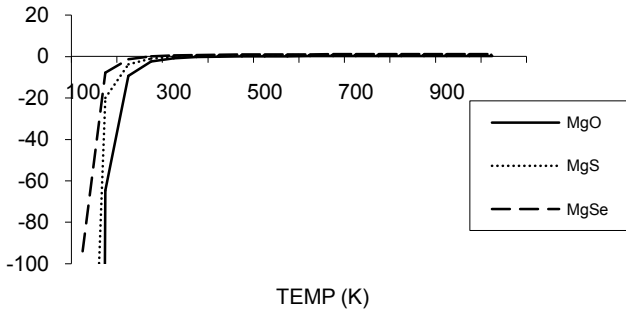

Figure 7. Variation of SOPD of C_{11} (in 10^{-11} N/m^2).

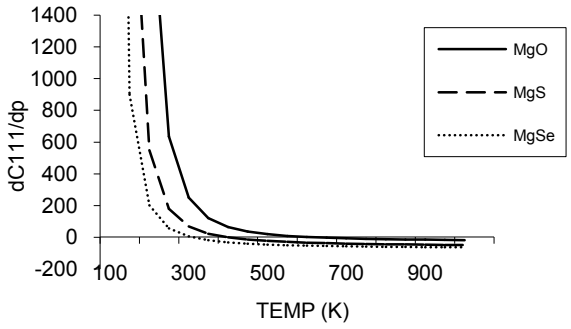

Figure 8. Variation of FOPD of C_{111} (in 10^{-11} N/m^2).