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Acoustical dissipation due to phonon-phonon interaction, thermoelastic loss and dislocation damping in MnO and CoO

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Temperature dependent ultrasonic attenuation due to phonon-phonon interaction, thermo-elastic mechanism and dislocation damping due to screw and edge dislocations have been evaluated in MnO and CoO in fcc (B1- type) phase, in a wide temperature range $50 \leq T \leq 500$ K for longitudinal and shear modes of propagation along three crystallographic directions viz. <100>, <110> and <111>. Electrostatic and Born-Mayer potentials were used to obtain second and third order elastic moduli at different temperatures taking interactions up to next nearest neighbours. Second and third order elastic moduli obtained at different temperatures have been used to obtain gruneisen parameters and non-linearity parameters which in turn were used to evaluate attenuation coefficient over frequency square viz. (α/f^2) for longitudinal and shear waves. Specific heat (as function of Debye temperature), hardness parameter and lattice parameter have been used as input data. Results have been discussed and it has been found that thermoelastic mechanism has negligible contribution to the total attenuation compared to phonon-phonon interaction.

1 Introduction

Transition metal oxides MnO and CoO are antiferromagnetic materials crystallize in to NaCl type (B1) structure. Predominant causes for ultrasonic attenuation (or sound attenuation) in solids are phonon-phonon interaction, electron-phonon interaction, thermoelastic loss and dislocation damping. At high temperatures, electron mean free path is not comparable to phonon mean free path, thus attenuation due to electron-phonon interaction is not present at higher temperatures. Therefore, phonon-phonon interaction, thermoelastic loss and dislocation damping are the dominant processes that will give rise the appreciable attenuation [1-3] beyond 50 K and above. Recently, electronic [4], phase transition [5] and elastic and pressure dependent acoustical properties [6] of MnO and CoO have been investigated extensively. In the present investigation, using simple potentials viz. electrostatic and repulsive potentials, second and third order elastic moduli (SOEM and TOEM) have been obtained at different temperatures, which in turn have been used to obtain sound attenuation and related parameters viz. Gruneisen parameters and non-linearity coupling constants over a wide temperature range.

2 Theoretical approach

2.1. Second and third order elastic moduli

According to Brugger's definition [7], n^{th} order elastic constant is defined as-

$$C_{ijklmn\ldots} = \left(\partial^n u / \partial\varepsilon_{ij}\partial\varepsilon_{kl}\partial\varepsilon_{mn}\ldots\ldots\right) \quad (1)$$

Where u is the crystal free-energy density and ε_{ij} is strain tensor.

Second and third order elastic moduli (SOEM and TOEM) at any temperature are obtained by adding corresponding vibrational contributions [7, 8], to SOEM & TOEM at absolute zero viz. C_{ij}^{0} &C_{ijk}^{0} i.e.

$$C_{ij}(T) = C_{ij}^{0} + C_{ij}^{vib.} \quad (2)$$

$$C_{ijk}(T) = C_{ijk}^{0} + C_{ijk}^{vib.} \quad (3)$$

Where $C_{ij}^{vib.}$ and $C_{ijk}^{vib.}$ are vibrational contribution to elastic constants. The explicit expressions are given in ref. [9].

2.2 Theory of ultrasonic attenuation

SOEM and TOEM are related by Gruneisen parameter γ_i^j and hence by non-linearity parameter, D. Ultrasonic attenuation due to phonon-phonon interaction for longitudinal and shear mode in Akhiezer regime ($\omega\tau << 1$) is given by [10-12]

$$(\alpha_{p-p})_l = \frac{2\pi^2 f^2 D_l E_0 \tau_l}{3dV_l^3} \quad (5)$$

$$(\alpha_{p-p})_s = \frac{2\pi^2 f^2 D_s E_0 \tau_s}{3dV_s^3} \quad (6)$$

Where non-linearity coupling constant (D) and thermal relaxation time (τ) are given by expressions [10-12]

$$D = 9\left\langle\left(\gamma_i^j\right)^2\right\rangle - \frac{3\left\langle\gamma_i^j\right\rangle^2 C_v T}{E_0} \quad (7)$$

$\left\langle \left(\gamma_i^{\,j}\right)^2 \right\rangle$ and $\left\langle \gamma_i^{\,j} \right\rangle$ are square average & average square Gruneisen parameters, V_l and V_s are sound wave velocity for longitudinal and shear waves respectively and d is density [10-12].

$$\tau = \tau_s = \frac{\tau_l}{2} = \frac{3K}{C_v < V >^2} \tag{8}$$

Where K is thermal conductivity, C_v is specific heat per unit volume and $< V >$ is Debye average velocity.

Propagation of sound wave through crystal produces compression and rarefactions as a result heat are transmitted from compressed region (at higher temperature) to rarefied region (at lower temperature) and hence thermoelastic loss occurs. Sound attenuation due to thermoelastic loss is given by [10-12].

$$(\alpha/f^2)_{th} = \frac{4\pi^2 \left\langle \gamma_i^{\,j} \right\rangle^2 KT}{2dV_L^{\,5}} \tag{9}$$

Debye average velocity is given by

$$\frac{3}{(< V >)^3} = \frac{1}{V_L^{\,3}} + \frac{2}{V_S^{\,3}} \tag{10}$$

The Debye temperature (which is used for obtaing C_v and E_0) is given by

$$\Theta_D = \hbar\, q_d <V> /K_B \tag{11}$$

Where is <V> Debye average velocity, K_B is Boltzmann constant and $q_d = (6\pi^2 n_a)^{1/3}$ where n_a is molar atomic concentration.

2.3 Attenuation by dislocation damping

Dislocation damping due to screw and edge dislocations also produces appreciable loss due to phonon-phonon interaction. The loss due to this mechanism can be obtained by multiplying dislocation viscosities by square of dislocation velocity. Viscous drag coefficient due to screw and edge dislocations is given by [12];

$$B_{screw} = 0.071\eta \tag{12a}$$

$$B_{edge} = 0.053\eta/(1-\sigma^2) + 0.0079/(1-\sigma^2)(\mu/B)\chi \tag{12b}$$

Where $\chi = \eta_1 - (4/3)\,\eta_s$, $\eta_1 = E_0 D_l \tau/3$, $\eta_s = E_0 D_s \tau/3$

$B = (C_{11} + 2C_{12})/3$, $\mu = (C_{11} - C_{12} + C_{44})/3$

and $\sigma = C_{12}/(C_{11} + C_{12})$

where B, μ, η, σ and χ are the bulk modulus, shear modulus, phonon viscosity, Poission's ratio and compressional viscosity respectively and C_{ij}'s are second order elastic moduli.

3 Results and discussions

Evaluated SOEM values are given in Table 1, together with the available experimental and theoretical values [4, 13-16]. These values are in good agreement with experimental and other theoretical values except minor disagreement in C_{12} and C_{44} values which may be attributed to the values of nearest neighbour distances (r) and hardness parameter (q), used by us.

Evaluated values of third order elastic moduli for MnO and CoO are given in Table 2. To the best of our knowledge, due to absence of experimental and theoretical data on third order elastic moduli, these have not been compared. In support of our calculated TOEM values, we have calculated TOEM values for NaCl by our programme and compared with TOEM values given in ref. [17], as shown in Table 2, which are of the same order and nearly have the same magnitude. Therefore, present TOEM values are justified.

Comp-ounds	C_{11} (10^{11} N/m^2)	C_{12} (10^{11} N/m^2)	C_{44} (10^{11} N/m^2)
MnO Present	2.23	1.32	0.38
Expt.	2.24 [14] 2.23[16]	1.14[14] 1.20[16]	0.78[14] 0.79[16]
Other	2.48[14], 2.20[15], 2.72[16]	1.38[14], 1.20[15], 1.28[16]	0.78[14], 1.38[15], 1.28[16]
CoO Present	2.77	1.38	0.42
Expt.	2.77[13], 2.56[14]	1.80[13], 1.44[14]	0.91[13], 0.84[14]
Other	2.77[17], 2.59[14], 2.17[16]	1.80[17], 1.67[14], 0.94[16]	0.91[17], 1.67[14], 0.94[16]

Table 1.Second order elastic constants of MnO and CoO at 300K

The sound velocity for longitudinal and shear waves (V_l and V_s), Debye average velocity (<V>), and

thermal relaxation time (τ) are given Table 3. They are compared with available data [6, 18] which are in good agreement with values obtained by others. On the basis of good agreement in V_l and V_s values it can be concluded that our second order elastic moduli values are satisfactory because V_l and V_s depend upon SOEM values [19].

Gruneisen parameters for MnO and CoO along [100] and [110] directions and different polarization are given in Table (4). Viscous drag coefficient due to screw and edge dislocations is given in Tables (5). Results are as expected since these have the same magnitude as other NaCl-type compounds [11, 12].

Comp-ounds	C_{111}	C_{112}	C_{123}	C_{144}	C_{166}	C_{456}
MnO	-42.23	-0.95	0.65	0.56	-1.37	0.64
CoO	-53.28	-1.11	0.78	0.77	-1.63	0.77
NaCl (Present	-9.17	-0.51	0.62	0.61	-0.11	0.61
Ref.[30]	-9.11	-0.91	0.34	0.26	-0.42	0.22

Table 2. Third order elastic constants (10^{11} N/m$^{2)}$ of MnO and CoO at 300K

Comp-ounds	V_l (10^3 m/sec)	Vs (10^3 m/sec)	<V> (10^3 m/sec)	τ (10^{-11} sec)
MnO Present	6.319	2.706	3.070	1.25
Other	6.439[8], 6.68[23]	3.820[8], 3.57[23]	------	-----
CoO Present	6.294	2.870	3.235	0.38
Other	6.323[8]	3.555[8]	------	------

Table .3. Ultrasonic velocity for longitudinal and shear wave V_l and V_s, Debye average velocity <V> and thermal relaxation time

Comp ounds	Direction of propagation	$<\gamma_i^{j2}>_l$	$<\gamma_i^j>^2_l$	$<\gamma_i^j>^2_s$	$<\gamma_i^j>^2_{s*}$
MnO	100	6.15	1.45	0.10	----
	110	5.54	1.81	0.47	12.76
CoO	100	6.41	1.47	0.09	----
	110	5.76	1.85	0.43	13.31

Table 4 Square Average and average square Gruneisen number for longitudinal $<\gamma_i^{j2}>_l$, $<\gamma_i^j>^2_l$ and shear $<\gamma_i^j>^2_s$, $<\gamma_i^j>^2_{s*}$ waves

Comp-ounds	Mode	Direction of propagation	Λ_{screw} (10^{-2} Poise)	Λ_{edge} (10^{-3} Poise)
MnO	Long.	100	0.61	0.55
		110	0.52	0.46
	Shear	100	0.11	0.29
		110	0.54	0.62
CoO	Long.	100	0.19	0.17
		110	0.16	0.14
	Shear	100	0.03	0.10
		110	0.14	0.18

Table .5. Viscous drag cofficients due to screw and edge dislocation for MnO and CoO at 300K longitudinal and shear (in poise) waves

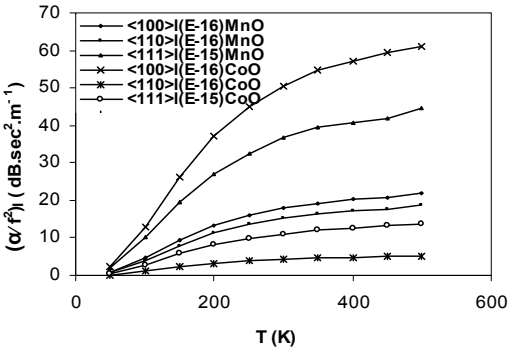

Fig.1.Temperature variation of $(\alpha/f^2)_l$ along diffrent directions of MnO and CoO.

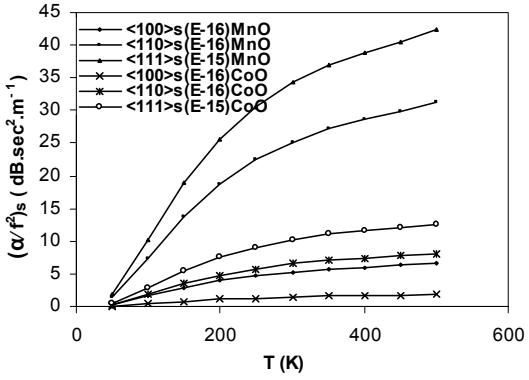

Fig. 2.Temperature variation of $(\alpha/f^2)_s$ along different directions of MnO and CoO

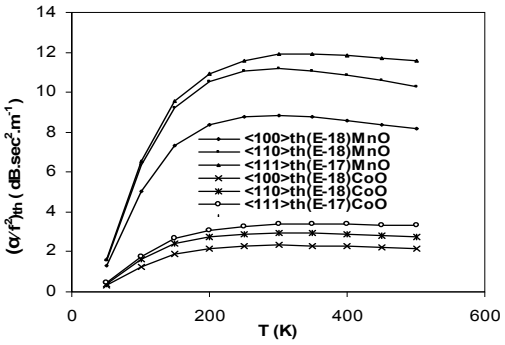

Fig.3 .Temperature variation of $(\alpha/f^2)_{th}$along different directions

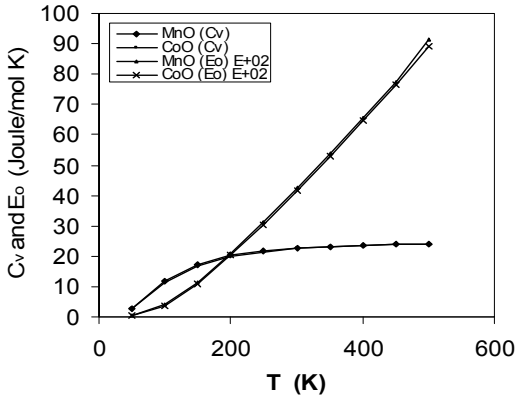

Fig.4. Temperature variation Specific heat C_v and energy density E_o of MnO and CoO

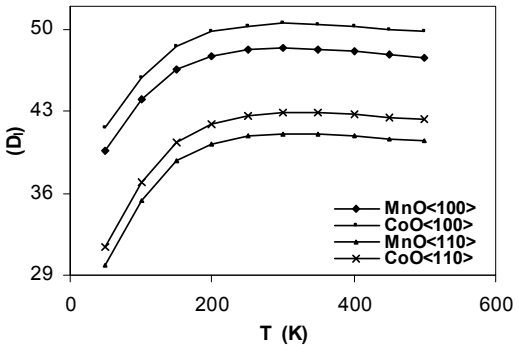

Fig. 5 Temperature variation acoustic coupling constant, D_l along [100] and [110] directions

Temperature variations of sound attenuation due to phonon-phonon interaction $((\alpha/f^2)_{p-p})$ for longitudinal and shear waves are shown in Figs. (1, 2). Figs. (1, 2) depict that temperature variation of ultrasonic attenuation has similar trend for longitudinal and shear wave and increases with

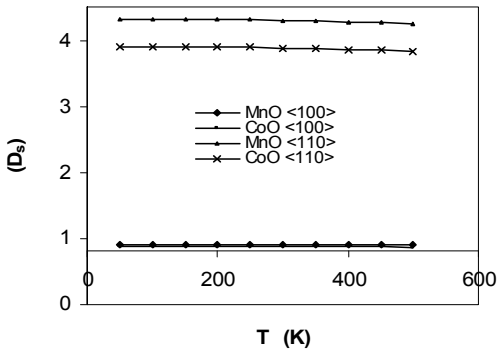

Fig. 6 Temperature variation acoustic coupling constant, D_s along [100] and [110] directions

temperature. $(\alpha/f^2)_{p-p}$ increases at faster rate due to increase of energy density, E_o at faster rate (Fig. 4). Temperature vs. E_o and C_v plots for MnO and CoO are overlapping due to nearly same values of Debye temperature (Θ_D = 425 and 440 for MnO and CoO respectively [15]), hence nearly same values of E_o and C_v (since Θ_D is function of E_o and C_v.).

Temperature variation of ultrasonic attenuation due to thermoelastic loss $((\alpha/f^2)_{th})$ for MnO and CoO is shown in Figs. (3). It increases up to 200 K and then becomes constant. This is due to fact that it is dominant by thermal conductivity (K), which depends on specific heat (since $K = 1/3\ C_V <V>^2 \tau$). The specific heat increases up to 200K and then it becomes constant at higher temperatures (Fig. 4). As specific heat increases, it gives large thermoelastic loss. When it becomes constant, thermoelastic loss becomes constant too, due to establishment of equilibrium state between compressional and rarefied regions.

Acoustic coupling constant is amount of acoustical energy converted into thermal energy. D_l increase with temperature up to 200 K and then becomes constant at higher temperatures while D_s remains almost constant (Fig. 5 and 6). Thus Attenuation in longitudinal wave is caused by (i) p-p interaction due to available energy density E_o and (ii) conversion of acoustical energy into thermal energy. Attenuation in shear wave is due to p-p interaction caused by E_o (since D_s remains constant)

4 Conclusions

Evaluated second and third order elastic moduli for MnO and CoO are in good agreement with the available results. Ultrasonic attenuation due to thermoelastic loss and dislocation damping due to screw and edge

dislocations is negligible in comparison to p-p interaction. Thus temperature dependent ultrasonic attenuation in these compounds is mainly governed by phonon-phonon interaction. ultrasonic attenuation due to phonon-phonon interaction for longitudinal and shear waves follows cube polynomial fit temperature dependent law and ultrasonic attenuation due to thermoelastic loss follows fourth order polynomial fit temperature dependent law in temperature range 50K-500K.

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