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, thermoelastic 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. $(\alpha/f^2)$ 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 crystalize 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:

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

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

Where $C_{ij}^0$ and $C_{ijk}^0$ 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 $\gamma'$ 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]

$$ (\alpha_{p-p})_l = \frac{2\pi^2 f^2 D_j E_{ij} \tau_i}{3dV^3} $$

$$ (\alpha_{p-p})_s = \frac{2\pi^2 f^2 D_j E_{ij} \tau_s}{3dV^3} $$

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

$$ D = 9 \left( \gamma'/T \right)^2 - \frac{3(\gamma'/T)^2 C_j T}{E_0} $$

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\( \langle p'_i p'_j \rangle \) and \( \langle p'_i p'_i \rangle \) 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].

\[
\tau = \tau_s = \frac{3K}{2C_s <V^2>}
\]

(8)

Where \( K \) is thermal conductivity, \( C_s \) 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].

\[
\frac{3}{<V>^3} = \frac{1}{V_l^3} + \frac{2}{V_s^3}
\]

(10)

Debye average velocity is given by

\[
\Theta_D = \frac{\hbar q_d <V>}{K_B}
\]

(11)

Where is \( <V> \) Debye average velocity, \( K_B \) is Boltzmann constant and \( q_d = (6\pi^2n_a)^{1/3} \) 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];

\[
B_{\text{screw}} = 0.071\eta
\]

(12a)

\[
B_{\text{edge}} = 0.053\eta(1-\sigma^2) + 0.0079/(1-\sigma^2)(\mu/B)\chi
\]

(12b)

Where \( \chi = \eta_1 - (4/3)\eta_s, \quad \eta_1 = E_0 D_t t/3, \quad \eta_s = E_0 D_s t/3 \)

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

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

where \( B, \mu, \eta, \sigma \) and \( \chi \) are the bulk modulus, shear modulus, phonon viscosity, Poisson’s ratio and compressional viscosity respectively and \( C_{ij} \) 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.

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

<table>
<thead>
<tr>
<th>Compounds</th>
<th>( C_{11} ) (10^11 N/m^2)</th>
<th>( C_{12} ) (10^11 N/m^2)</th>
<th>( C_{44} ) (10^11 N/m^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnO Present</td>
<td>2.23</td>
<td>1.32</td>
<td>0.38</td>
</tr>
<tr>
<td></td>
<td>2.23[16]</td>
<td>1.20[16]</td>
<td>0.79[16]</td>
</tr>
<tr>
<td>Other</td>
<td>2.48[14], 2.20[15], 2.72[16]</td>
<td>1.38[14], 1.20[15], 1.28[16]</td>
<td>0.78[14], 1.38[15], 1.28[16]</td>
</tr>
<tr>
<td>CoO Present</td>
<td>2.77</td>
<td>1.38</td>
<td>0.42</td>
</tr>
<tr>
<td>Expt.</td>
<td>2.77[13], 2.56[14]</td>
<td>1.80[13], 1.44[14]</td>
<td>0.91[13], 0.84[14]</td>
</tr>
<tr>
<td>Other</td>
<td>2.77[17], 2.59[14], 2.17[16]</td>
<td>1.80[17], 1.67[14], 0.94[16]</td>
<td>0.91[17], 1.67[14], 0.94[16]</td>
</tr>
</tbody>
</table>

The sound velocity for longitudinal and shear waves (\( V_l \) and \( V_s \)), Debye average velocity (<\( V >\)), and...
thermal relaxation time ($\tau$) 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].

<table>
<thead>
<tr>
<th>Compounds</th>
<th>$C_{111}$</th>
<th>$C_{112}$</th>
<th>$C_{123}$</th>
<th>$C_{144}$</th>
<th>$C_{166}$</th>
<th>$C_{456}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnO</td>
<td>-42.23</td>
<td>-0.95</td>
<td>0.65</td>
<td>0.56</td>
<td>-1.37</td>
<td>0.64</td>
</tr>
<tr>
<td>CoO</td>
<td>-53.28</td>
<td>-1.11</td>
<td>0.78</td>
<td>0.77</td>
<td>-1.63</td>
<td>0.77</td>
</tr>
<tr>
<td>NaCl (Present)</td>
<td>-9.17</td>
<td>-0.51</td>
<td>0.62</td>
<td>0.61</td>
<td>-0.11</td>
<td>0.61</td>
</tr>
<tr>
<td>Ref.[30]</td>
<td>-9.11</td>
<td>-0.91</td>
<td>0.34</td>
<td>0.26</td>
<td>-0.42</td>
<td>0.22</td>
</tr>
</tbody>
</table>

Table 2. Third order elastic constants ($10^{13}$ N/m$^2$) of MnO and CoO at 300K

<table>
<thead>
<tr>
<th>Compounds</th>
<th>Mode</th>
<th>Direction of propagation</th>
<th>$\Lambda_{\text{Screw}}$ ($10^{-2}$ Poise)</th>
<th>$\Lambda_{\text{Edge}}$ ($10^{-3}$ Poise)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnO</td>
<td>Long.</td>
<td>100</td>
<td>0.61</td>
<td>0.55</td>
</tr>
<tr>
<td></td>
<td></td>
<td>110</td>
<td>0.52</td>
<td>0.46</td>
</tr>
<tr>
<td></td>
<td>Shear</td>
<td>100</td>
<td>0.11</td>
<td>0.29</td>
</tr>
<tr>
<td></td>
<td></td>
<td>110</td>
<td>0.54</td>
<td>0.62</td>
</tr>
<tr>
<td>CoO</td>
<td>Long.</td>
<td>100</td>
<td>0.19</td>
<td>0.17</td>
</tr>
<tr>
<td></td>
<td></td>
<td>110</td>
<td>0.16</td>
<td>0.14</td>
</tr>
<tr>
<td></td>
<td>Shear</td>
<td>100</td>
<td>0.03</td>
<td>0.10</td>
</tr>
<tr>
<td></td>
<td></td>
<td>110</td>
<td>0.14</td>
<td>0.18</td>
</tr>
</tbody>
</table>

Table 4 Square Average and average square Gruneisen number for longitudinal $<\gamma_i^2>_L$ and shear $<\gamma_i^2>_S$, $<\gamma_i>'^2$, waves

<table>
<thead>
<tr>
<th>Compounds</th>
<th>Mode</th>
<th>Direction of propagation</th>
<th>$\Lambda_{\text{Screw}}$ ($10^{-2}$ Poise)</th>
<th>$\Lambda_{\text{Edge}}$ ($10^{-3}$ Poise)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnO</td>
<td>Long.</td>
<td>100</td>
<td>0.61</td>
<td>0.55</td>
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<td></td>
<td></td>
<td>110</td>
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<td>Shear</td>
<td>100</td>
<td>0.11</td>
<td>0.29</td>
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<td></td>
<td>110</td>
<td>0.54</td>
<td>0.62</td>
</tr>
<tr>
<td>CoO</td>
<td>Long.</td>
<td>100</td>
<td>0.19</td>
<td>0.17</td>
</tr>
<tr>
<td></td>
<td></td>
<td>110</td>
<td>0.16</td>
<td>0.14</td>
</tr>
<tr>
<td></td>
<td>Shear</td>
<td>100</td>
<td>0.03</td>
<td>0.10</td>
</tr>
<tr>
<td></td>
<td></td>
<td>110</td>
<td>0.14</td>
<td>0.18</td>
</tr>
</tbody>
</table>

Table 5. Viscous drag coefficients 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 different directions of MnO and CoO.](image1.png)

![Fig.2.Temperature variation of ($\alpha/f^2$)$_s$ along different directions of MnO and CoO.](image2.png)
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 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 \(\Theta_D = 425\) and \(440\) for MnO and CoO respectively [15]), hence nearly same values of \(E_o\) and \(C_v\) (since \(\Theta_D\) 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.

Reference


