Ultrasonic Properties of Hexagonal Closed Packed Metals

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Abstract This work is focused on three types of ultrasonic velocities (V_1 , V_2 and V_3) in Mg and Cd hcp metals. These are determined using the SOEC and TOEC at room temperature. Ultrasonic waves were supposed to be propagated along different directions with the crystal axis (z-axis). Finally ultrasonic attenuation in Mg and Cd are evaluated at room temperature utilizing the SOEC and TOEC of the materials. Average wave velocity is highest at $\theta=55^\circ$ along z-axis in these materials. The contributions of the elastic constants, thermal conductivity, thermal energy density, ultrasonic velocity and acoustic coupling constant to the total attenuation are studied.

Keywords Ultrasonic Velocity, Acoustic Coupling Constant, Ultrasonic Attenuation

1. Introduction

Magnesium and Cadmium are hexagonal close packed structured metal. As with other related rare earth metals, these are malleable, ductile and lustrous silvery white metals. Magnesium chloride is present in sea water. It is widely distributed in the vegetable kingdom being present in chlorophyll, the green coloured pigment in leaves. Magnesium is not tarnished in dry air. In contact with wet air, a thin layer of oxide is coated on the metal surface. In flash light photography, Mg wire burns with dazzling light in an atmosphere of oxygen. The light is rich in ultraviolet radiations. Magnesium is used as an alloying agent in producing Magnalium, which is extensively used in the construction of aeroplanes, motors, and balance beams light instruments. Being highly electropositive in nature, it is used for sacrificial protection of iron pipelines, piers and ships against corrosion. It is also used as deoxidiser for removing last traces of oxygen from copper, steel, etc.

Cadmium is white, lustrous, but tarnishable metal. Their

structure deviates only slightly from perfect hcp. Cadmium is remarkably volatile for heavy metals. The elements have relatively low abundance in nature (of the order 10^{-6} of earths crust for Cd.), but have long been known because this is easily obtained from their ores. Cadmium is very electro positive and react readily with nonoxidizing acids releasing H_2 and giving the divalent ions. The element Cd. from many alloys. Cadmium is mostly found isomorphously replacing zinc in zinc minerals. It is also used the low efficiency of nuclear reactor.

There is a plenty (abundant) of literature on behaviour of elastic constant and thermal properties of these metals [1-7], but the studies on ultrasonic propagating behaviour in these materials are not reported in literature. The aim of present chapter is to establish the theory of for determination of ultrasonic attenuation, ultrasonic velocity, thermal relaxation time and other related parameters like non-linearity constants (acoustic coupling constants) in the materials at 300K.

In the present paper three types of ultrasonic velocities (V_1 , V_2 and V_3) in Mg and Cd are determined using the SOEC and TOEC at room temperature. Ultrasonic waves were supposed to be propagated along different directions with the crystal axis (z-axis). Finally ultrasonic attenuation in Mg and Cd are evaluated at room temperature utilizing the SOEC and TOEC of the materials. Acoustic coupling constants (non-linearity constants) and thermal relaxation time are determined for the determination of ultrasonic attenuation.

2. Theory: Theoretical Description is Categorized into Two Parts

2.1. Ultrasonic Velocity In Hcp Crystal

There are three types of ultrasonic velocities in hcp crystals as one longitudinal and two shear wave velocities, which are given by the following expressions [8-11].

$$V_1^2 = \{C_{33} \cos^2 \theta + C_{11} \sin^2 \theta + C_{44} + \{[C_{11} \sin^2 \theta - C_{33} \cos^2 \theta + C_{44}(\cos^2 \theta - \sin^2 \theta)]^2\}$$

$$+ 4 \cos^2 \theta \sin^2 \theta (C_{13} + C_{44})^2 \}^{1/2} \} / 2\rho \quad (1)$$

$$V_2^2 = \{C_{33} \cos^2 \theta + C_{11} \sin^2 \theta + C_{44} - \{[C_{11} \sin^2 \theta - C_{33} \cos^2 \theta + C_{44}(\cos^2 \theta - \sin^2 \theta)]^2 + 4 \cos^2 \theta \sin^2 \theta (C_{13} + C_{44})^2 \}^{1/2} \} / 2\rho \quad (2)$$

$$V_3^2 = \{C_{44} \cos^2 \theta + C_{66} \sin^2 \theta\} / \rho \quad (3)$$

Where V_1 , V_2 and V_3 are the longitudinal, quasi-shear and shear wave velocities. The ρ and θ are the density of the material and angle with the unique axis (z-axis) of the crystal. C_{11} , C_{13} , C_{33} , C_{44} and C_{66} are the second order elastic constants (SOEC) of the material.

The room temperature properties of the crystals are commonly characterized by Debye average velocity. This is determined as the mean (Debye) sound velocity ($\bar{V}$), which is calculated from the initial slopes of the three acoustical branches [12-13].

$$\bar{V} = \left(\frac{1}{3} \sum_{i=1}^3 \int \frac{1}{V_i^3} \frac{d\Omega}{4\pi} \right)^{-1/3} \quad (4)$$

The integration is over all directions and the summation is over the three acoustic branches (V_i).

2.2. Ultrasonic Attenuation

According to Mason [14], the two dominant processes that will give rise to appreciable ultrasonic attenuation in hexagonal structured materials at high temperatures are phonon-phonon interaction also known as Akhieser loss and that due to thermo-elastic attenuation. The ultrasonic attenuation coefficient $(\alpha)_{\text{Akh}}$ (Akhieser type loss) due to phonon-phonon interaction mechanism is given by following expression [14-17].

$$(\alpha)_{\text{Akh}} = \omega^2 \Delta C \tau / 2 \rho V^3 (1 + \omega^2 \tau^2) \quad (5)$$

where ω is angular frequency of the wave and V is the velocity of ultrasonic wave (longitudinal and shear). τ is the thermal relaxation time whose expression is as:

$$\tau = \tau_S = \tau_L / 2 = 3 K / C_V \bar{V}^2 \quad (6)$$

Here τ_L and τ_S are the thermal relaxation time for longitudinal and shear wave. K and C_V are the thermal conductivity and specific heat per unit volume of the material. ΔC is change in elastic modulus caused by strain and is given by:

$$\Delta C = 3E_0 < (\gamma_i^j)^2 > - < \gamma_i^j >^2 C_V T = E_0 D / 3 \quad (7)$$

Where E_0 is thermal energy density and γ_i^j Grüneisen number: i, j are the mode and direction of propagation.

The propagation of longitudinal ultrasonic wave creates

compression and rarefaction throughout the lattice. The rarefied regions are colder than that of the compressed region. Thus there is flow of heat between these two regions. Hence thermo-elastic loss $(\alpha)_{\text{th}}$ occurs and is given by [16-17].

$$(\alpha)_{\text{th}} = \omega^2 < \gamma_i^j >^2 K T / 2 \rho V_1^5 \quad (8)$$

The calculations have been carried out both manually and a computer program in MATLAB, which is based on formulae given in paper. The program has been confirmed and verified with previous calculations.

3. Results and Discussion

The values of second and third order elastic constants for Mg and Cd are taken from literature [6-7] and are presented in the Table 1. The value of density (ρ) and thermal conductivity K at 300K are taken from the physical constant table. The value of specific heat per unit volume (C_V) and thermal energy density (E_0) are evaluated using physical constant table and Debye temperature [18]. The values of K , ρ , C_V and E_0 are presented in Table2.

Table 1. SOEC and TOEC in 10^{10}N/m^2 for Mg and Cd at 300 K.

SOEC/TOEC	Mg	Cd
C_{11}	5.943	1.158
C_{12}	2.560	3.975
C_{13}	2.140	4.06
C_{33}	6.146	5.14
C_{44}	1.642	2.039
C_{66}	1.691	3.801
C_{111}	-64.300	-2.448
C_{112}	-17.900	-7.91
C_{113}	-6.300	-1.71
C_{123}	-4.700	-7.3
C_{133}	-17.100	-2.0
C_{144}	-4.500	-6.8
C_{155}	-6.500	-1.76
C_{222}	-73.700	-2.92
C_{333}	-63.200	-6.67
C_{344}	-17.100	-2.0

Table 2. Thermal conductivity K ($\text{Wm}^{-1}\text{K}^{-1}$), density ρ (10^3 Kg m^{-3}), specific heat per unit Vol. C_V ($10^6 \text{ Jm}^{-3} \text{ K}^{-1}$), thermal energy density E_0 (10^8 Jm^{-3}), for Mg and Cd at 300K.

Physical constants	Mg	Cd
K	156.00	970
ρ	1.740	3.65
C_V	1.641	1.881
E_0	3.155	4.416

The three ultrasonic velocities V_1 , V_2 and V_3 are

Figure 1. Longitudinal velocity (V_1) Vs. angle with z-axis

Figure 2. Quasi shear velocity (V_2) Vs. angle with z-axis

calculated using the second order elastic constants and the Eqs. (1)-(3) at 300K and different angles with the unique axis (z-axis) of the crystal. The obtained values of velocities are presented in Table 3 and Figures. 1-3. The thermal relaxation time (τ) is calculated at different angles with unique axis of the crystal. The present values of τ and $\bar{V}$ are given in Table 4. The angle dependency of thermal relaxation time is shown in Figure 4. The Grüneisen numbers are calculated by the expressions given by Nandanpawar et al. [19] at 300K taking $\theta=0^\circ$. The Grüneisen numbers and acoustic coupling constants are presented in Table 5.

Figure 3. Shear velocity (V_3) Vs. angle with z-axis

Figure 4. Thermal relaxation time (τ) Vs. angle with z-axis

Table 3. Velocity (V_1 , V_2 , and V_3) at different angles (θ) from Z-axis for Mg and Cd at 3000K.

Metal →	Mg	Cd	Mg	Cd	Mg	Cd
θ	V_1	V_1	V_2	V_2	V_3	V_3
0	5.952	2.437	3.072	1.535	3.072	1.535
5	5.947	2.453	3.080	1.528	3.072	1.540
15	5.910	2.567	3.139	1.485	3.075	1.579
25	5.847	2.749	3.232	1.438	3.080	1.649
35	5.783	2.957	3.317	1.416	3.087	1.740
45	5.743	3.162	3.353	1.422	3.095	1.837
55	5.743	3.345	3.321	1.450	3.103	1.930
65	5.774	3.494	3.237	1.485	3.110	2.008
75	5.814	3.598	3.142	1.515	3.115	2.063
85	5.841	3.652	3.080	1.533	3.118	2.093
90	5.844	3.658	3.072	1.535	3.118	2.096

Table 4. Debye average elocity (10^3 m/sec) and relaxation time τ_{th} (10^{-12} s) at different angles (θ) from Z-axis for Mg and Cd at 300 K.

Metal→	Mg		Cd	
θ	$\bar{V}$	τ_{th}	$\bar{V}$	τ_{th}
0	3.396	0.2473	1.669	5.549
5	3.400	0.2467	1.669	5.547
15	3.430	0.2424	1.672	5.527
25	3.474	0.2363	1.683	5.459
35	3.513	0.2310	1.708	5.031
45	3.532	0.2287	1.749	5.052
55	3.523	0.2298	1.802	4.758
65	3.490	0.2342	1.856	4.488
75	3.448	0.2399	1.899	4.289
85	3.419	0.2440	1.922	4.186
90	3.415	0.2445	1.925	4.173

A perusal of Figure 1 shows that a minimum of longitudinal velocity (V_1) is found at 55° with the unique axis for Mg, it decreases with angle while velocity increases for Cd. Figure 2 shows that quasi shear velocity (V_2) has maximum value for Mg and minimum for Cd at 45° . Figure 3 shows that the pure shear velocity (V_3) slightly increases for Mg and Cd with the angle. All the anomalous behaviour in

three type of velocity in these metals is due to anomalous values of the second order elastic constants (SOEC), which is the direct consequence of the crystal anisotropy. Figures 1-3 demonstrate that V_1 has minimum value for Mg at 55° while increasing value of Cd, V_2 is maximum for Mg and minimum for Cd at 45° and V_3 is maximum for Mg and Cd both at 90° .

Figure 4 shows that if ultrasonic wave is supposed to propagate along different angles with the unique axis then the time for reestablishment of thermal phonons equilibrium decreases from 0° - 35° and shows a minimum at 45° and increases from 55° - 90° for Mg but in case of Cd it decreases from 0° - 90° and shows a maximum at 0° and minimum 90° . Debye average velocity is affecting factor for the anomalous nature of relaxation time. The reestablishment of thermal phonons (relaxation time) is maximum when ultrasonic wave is propagated along $\theta=0^\circ$ with the unique axis of the crystal.

Table 5. Average Gruneisen number $\langle \gamma_i^j \rangle_L$, square of average Gruneisen number $\langle (\gamma_i^j)^2 \rangle_L$ for longitudinal wave, average square Gruneisen number $\langle (\gamma_i^j)^2 \rangle_L$ and $\langle (\gamma_i^j)^2 \rangle_S$ for longitudinal and shear wave and non-linearity constants D_L , D_S for longitudinal and shear wave along Z-axis for Mg and Cd at 300°K .

Parameter s	Mg	Cd	Ti [21]	Zr [21]	Hf [21]
$\langle \gamma_i^j \rangle_L$	-1.0125	82.769			
$\langle (\gamma_i^j)^2 \rangle_L$	1.0251	2.771			
$\langle (\gamma_i^j)^2 \rangle_S$	22.2209	6.850			
$\langle (\gamma_i^j)^2 \rangle_S$	0.1299	1.653			
D_L	195.1897	2.468	55.965	56.314	56.521
D_S	1.1694	1.487	1.406	1.249	1.418

The ultrasonic attenuation coefficient $(\alpha/f^2)_{Akh}$ for longitudinal and shear wave are calculated at 300K taking $\theta=0^\circ$ Thermoelastic loss $(\alpha/f^2)_{th}$ is also calculated at 300K taking $\theta=0^\circ$. The values of $(\alpha/f^2)_{Akh}$ and $(\alpha/f^2)_{th}$ are presented in Table 6.

Table 6. Ultrasonic attenuation coefficient $(\alpha/f^2)_{Akh}$ in $10^{-14}\text{NpS}^2\text{m}^{-1}$ and thermoelastic attenuation coefficient $(\alpha/f^2)_{th}$ in $10^{-16}\text{NpS}^2\text{m}^{-1}$ for longitudinal and shear waves along Z-axis ($\theta=0^\circ$) for Mg and Cd at 300°K and 10MHz.

Metal	$(\alpha/f^2)_{Akh, \text{long.}}$	$(\alpha/f^2)_{Akh, \text{shear}}$	$(\alpha/f^2)_{th}$
Mg	10.915	23.80	7280.0
Cd	0.0127	0.0016	0.0006

Grüneisen parameter plays a significant role in study of thermoelastic properties of materials. It is used to describe physical properties of the materials. The SOEC and TOEC are used to obtain Grüneisen numbers expressions as given in literature[19]. The average Grüneisen parameter of Cd is more than Mg as shown in Table 5. So we can say that Cd is

stronger candidate than Mg for thermoelastic purpose [20]. The acoustic coupling constant (D) is measure of acoustic energy converted into thermal energy under relaxation process. A comparison for D has been made in Table 5 with hcp lanthanide metals [21]. The obtained results are more or less similar to them.

Here, a theoretical calculation is done for ultrasonic attenuation in hcp metals Mg and Cd. The above discussion implies that the characteristic values of V_1 , V_2 and V_3 of Mg metal are correlated with the second order elastic constants. The orientation dependent relaxation time is mainly affected by Debye average velocity. The ultrasonic attenuation for longitudinal wave is predominantly affected by thermal energy density and mass density of the metal and the ultrasonic attenuation for shear wave is predominantly affected by the shear wave velocity and relaxation time. The longitudinal wave velocity is the dominating property for the thermoelastic loss. By these informations, the anisotropic behaviour and characteristic features of this material can be understood and the results obtained by present theoretical approach are informative for the understanding of basic properties of this hcp metal Mg.

4. Conclusion

On the basis of above discussion, we conclude following points:

1. Average ultrasonic velocity increases from $\theta=0^\circ$ to 55° , then it decreases from $\theta=55^\circ$ to 90° in these metals. Hence it is maximum at 55° along z-axis.
2. Thermal relaxation time (τ) decreases first from 0° - 45° , then it increases from 45° - 90° (in case of Mg) while it decreases continuously in case of Cd like a relaxation $\tau=\tau_0\exp(-\lambda/T)$.
3. Acoustic coupling constant (D) of Mg for longitudinal wave is more, while it is less for Cd.
4. Ultrasonic attenuation due to phonon-phonon interaction mechanism is predominant over thermoelastic loss.

Obtained results of present investigation can be used for further investigation and industrial applications.

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