

23]. It is also reported by the previous workers that ultrasonic shear wave velocity is more sensitive for the study of the basic properties [14].

In the present investigation, ultrasonic attenuation as a function of temperature due to phonon-phonon interaction is studied in Copper (Cu), Silver (Ag) and Gold (Au) at different temperatures, viz. 100, 200, 300 and 400 K, using repulsive parameter ( $q$ ), interatomic distance ( $r$ ) and Born-Mayer [24] potentials following Mason's approach [13]. The thermal relaxation time, average Gruneisen parameters, non-linearity constants and attenuation coefficients for longitudinal and shear waves are evaluated along  $\langle 100 \rangle$  direction of propagation.

## 2. Theory

As present study is concerned with attenuation coefficients at different temperatures, the third order elastic constants are required at these specific temperatures. Third order elastic constants (TOECs) are evaluated using Born-Mayer potential,  $Q(r) = A \exp(-r/q)$  and Coulomb potential,  $\pm e^2/r$ , ( $r, q$  and  $e$  being interatomic distance, hardness parameter and electronic charge, respectively). According to Brugger's [25] definition for elastic constants, one obtains the three expressions for TOECs at absolute zero temperature, given in Table 1.

**Table 1.** Expressions for the third order elastic constants at 0K.

$$C_{111}^0 = 10.2639G - G_3 - 2G_4,$$

$$C_{112}^0 = C_{166}^0 = 1.208625G - G_4,$$

$$C_{123}^0 = C_{144}^0 = C_{456}^0 = 0.678375G.$$

### Expressions for G's

$$G = e^2/r_0^4, G_1 = (1/r_0 + 1/q) Q (or)/qr_0,$$

$$G_2 = (\sqrt{2}/2r_0 + 1/q) Q (r_0 \sqrt{2})/qr_0,$$

$$G_3 = (3/r_0^2 + 3/qr_0 + 1/q^2) Q (r_0)/q,$$

$$G_4 = (3\sqrt{2}/r_0^2 + 6/qr_0 + 2\sqrt{2}/q^2) Q (r_0 \sqrt{2})/4q,$$

$$G_5 = (15/r_0^3 + 15/qr_0^2 + 6/q^2r_0 + 1/q^3) r_0 Q (r_0)/q,$$

$$G_6 = (15\sqrt{2}/4r_0^3 + 15/2qr_0^2 + 3\sqrt{2}/q^2r_0 + 1/q^3) r_0 Q (r_0 \sqrt{2})/2q.$$

Seeger and Mann [26] has already studied these crystals and obtained the second order elastic constants (SOECs) using the same potentials. The temperature dependence of elastic constants is determined using anharmonicity theory of crystal dynamics developed by Leibfried and Hahn [27] or Leibfried and Ludwig [28] given below :

$$C_{\mu\nu}(T) = C_{\mu\nu}^0 + C_{\mu\nu} T, \quad (1)$$

where

$$C_{ijk} = I_1 K (\partial C_{ijk}^0 / \partial r)_{r=r_0} + C_{ijk}^{vib} \quad (2)$$

$I_1$  is a function of hardness parameter and interatomic distance given by

$$I_1 = -q \left\{ (2 + 2q_0 - q_0^2) Q(r_0) + 2\sqrt{2}(1 + 2q_0 - q_0^2) Q(r_0\sqrt{2}) \right\} / I_2 \quad (3)$$

and

$$I_2 = 2 \left\{ (q_0 - 2) Q(r_0) + 2(q_0 - \sqrt{2}) Q(r_0\sqrt{2}) \right\} \times \left\{ (q_0 - 2) Q(r_0) + 4(q_0 - \sqrt{2}) Q(r_0\sqrt{2}) \right\} \quad (4)$$

**Table 2.** Expressions for vibrational contribution to the third order elastic constants.

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$$C_{111}^{vib} = g_3 F_1^3 + g_2 F_2 F_1 + g_1 G_3,$$

$$C_{112}^{vib} = g_1 F_1^3 + g_2 F_1 (2F_5 + F_2) + g_1 F_6,$$

$$C_{123}^{vib} = g_3 F_1^3 + 3g_2 F_1 F_5,$$

$$C_{144}^{vib} = g_2 F_1 F_5,$$

$$C_{166}^{vib} = g_2 F_1 F_5 + g_1 F_6,$$

$$C_{456}^{vib} = 0.$$

**Table 3.** Expressions for  $g_n$  for highly conducting metals.

$$g_1 = g_0 S;$$

$$g_2 = g_0 [(X / S_1) + S] / 2;$$

$$g_0 = h\omega_0 / 8r_0^3;$$

$$g_3 = g_0 [(2X^2 S / 3S_1) + (X / S_1) + S] / 48;$$

$$X = h\omega_0 / 2KT;$$

$$g_4 = -g_0 [(X^3 S^2 / 3S_1) + (X^3 / 6S_1^2) + (X^2 S / S_1) + (5X / 4S_1) + (5S / 4)] / 144;$$

$$\omega_0 = (1 / M^+ + 1M^-) / qr_0 F_0;$$

$$S = \text{Coth } X, \quad S_1 = \text{Sinh}^2 X$$


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and  $C_{ijk}^{vib}$  are the contributions due to vibrational energy of the crystal and these values are given in Table 2. The expressions of different  $G_n$ 's and  $F_n$ 's are shown in Table 3 and 4. Mason [13] has shown that the Gruneisen numbers are related with the second and third order elastic constants. Therefore, the Gruneisen numbers  $\gamma_i'$  are evaluated using Gruneisen tables [13], and second and third order elastic constants are thus obtained. The

non-linearity constant [13] 'D' is related to Gruneisen numbers as

$$D = 9 \langle \gamma_i'^2 \rangle - (3CT \langle \gamma_i' \rangle^2) / E, \quad (5)$$

where  $C$ ,  $T$  and  $E$  are specific heat, absolute temperature and energy of the crystal, respectively;  $\langle \gamma_i'^2 \rangle$  and  $\langle \gamma_i' \rangle$  are square average and simple average of Gruneisen numbers.

One gets the following relations for phonon viscosity and thermoelastic losses [13] using Gruneisen numbers and non linearity constants.

$$(\alpha / f^2)_{p-p} = (2\pi)^2 ED\tau_m / 3dV^3(1 + \omega^2\tau_m^2), \quad (6)$$

$$(\alpha / f^2)_m = (2\pi)^2 \langle \gamma_i' \rangle^2 KT / 2dV^5, \quad (7)$$

where 'K' is the thermal conductivity, 'd' the density of the substance, ' $\omega$ ' ( $=2\pi f$ ) the angular frequency of the ultrasonic wave and ' $\tau_m$ ' the thermal relaxation time for the exchange of acoustic and thermal energies, given by

$$\frac{1}{2}\tau_1 = \tau_s = \tau_m = 3K / C\bar{V}^2 \quad (8)$$

'V' represents  $V_l$  (longitudinal wave velocity) or  $V_s$  (shear wave velocity) and  $\bar{V}$  is the Debye average velocity. These are computed according to the relations :

$$V_l = (C_{11} / d)^{\frac{1}{2}},$$

$$V_s = (C_{44} / d)^{\frac{1}{2}},$$

$$3/\bar{V}^3 = 1/V_l^3 + 2/V_s^3. \quad (9)$$

As the whole evaluation is based upon elastic constants and these elastic constants are obtained using repulsive parameter and interatomic distance of the crystal, one may successfully conclude that attenuation is one of the basic properties of substance.

**Table 4.** Expressions for  $F_n$  for highly conducting metals.

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$$F_0 = 1/(q_0 - 2) Q(r_0) + 2(q_0 - \sqrt{2}) Q(r_0\sqrt{2})$$

$$q_0 = r_0/q;$$

$$F_1 = 2[(2 + 2q_0 - q_0^2) Q(r_0) + 2(\sqrt{2} + 2q_0 - \sqrt{2}q_0^2) Q(r_0\sqrt{2})] F_0;$$

$$F_2 = 2(-6 - 6q_0 - q_0^2 + q_0^3) Q(r_0) F_0 + F_1;$$

$$F_3 = 2(-30 - 30q_0 - 9q_0^2 + q_0^3 - q_0^4) Q(r_0) F_0 + F_1;$$

$$F_4 = 2(-210 - 210q_0 - 75q_0^2 - 5q_0^3 + 4q_0^4 + q_0^5) Q(r_0) F_0 + F_1 + F_2;$$

$$F_5 = (-3\sqrt{2} - 6q_0 - \sqrt{2}q_0^2 + 2q_0^3) Q(r_0\sqrt{2}) F_0;$$

$$F_6 = [(15/\sqrt{2}) + 15q_0 - (9/\sqrt{2})q_0^2 - 9q_0^3 - \sqrt{2}q_0^4] Q(r_0\sqrt{2}) F_0;$$

$$F_7 = [-(105/2\sqrt{2}) - 105/2] q_0 - (75/2\sqrt{2}) q_0^2 - (5/2) q_0^3 + 2\sqrt{2} q_0^4 + q_0^5] Q(r_0\sqrt{2}) F_0.$$

### 3. Evaluation

According to Tables 1-4, the third order elastic constants are evaluated at different temperatures using hardness parameter [26] and nearest neighbour distance [29]. Taking second order elastic constants from literature [29, 30] and calculated third order elastic constants, average Gruneisen numbers  $\langle \gamma_l'^2 \rangle$  and  $\langle \gamma_l' \rangle$  are evaluated along  $\langle 100 \rangle$  direction of propagation for longitudinal and shear waves using Manson's Gruneisen [13] Tables (Table 5). The thermal relaxation time ' $\tau_{th}$ ' is computed using thermal conductivity

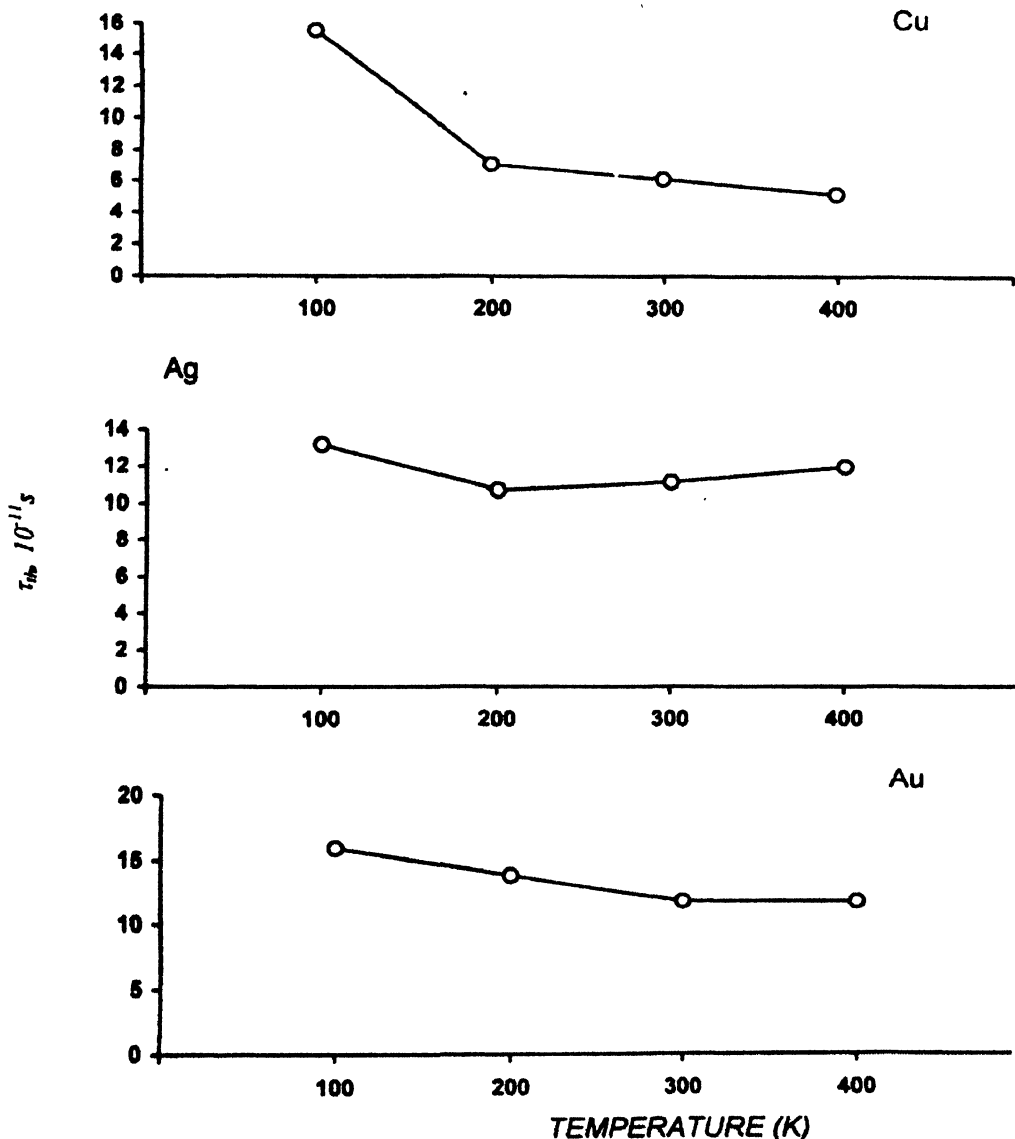


Figure 1. Temperature dependence of thermal relaxation time in  $\langle 100 \rangle$  highly conducting metals.

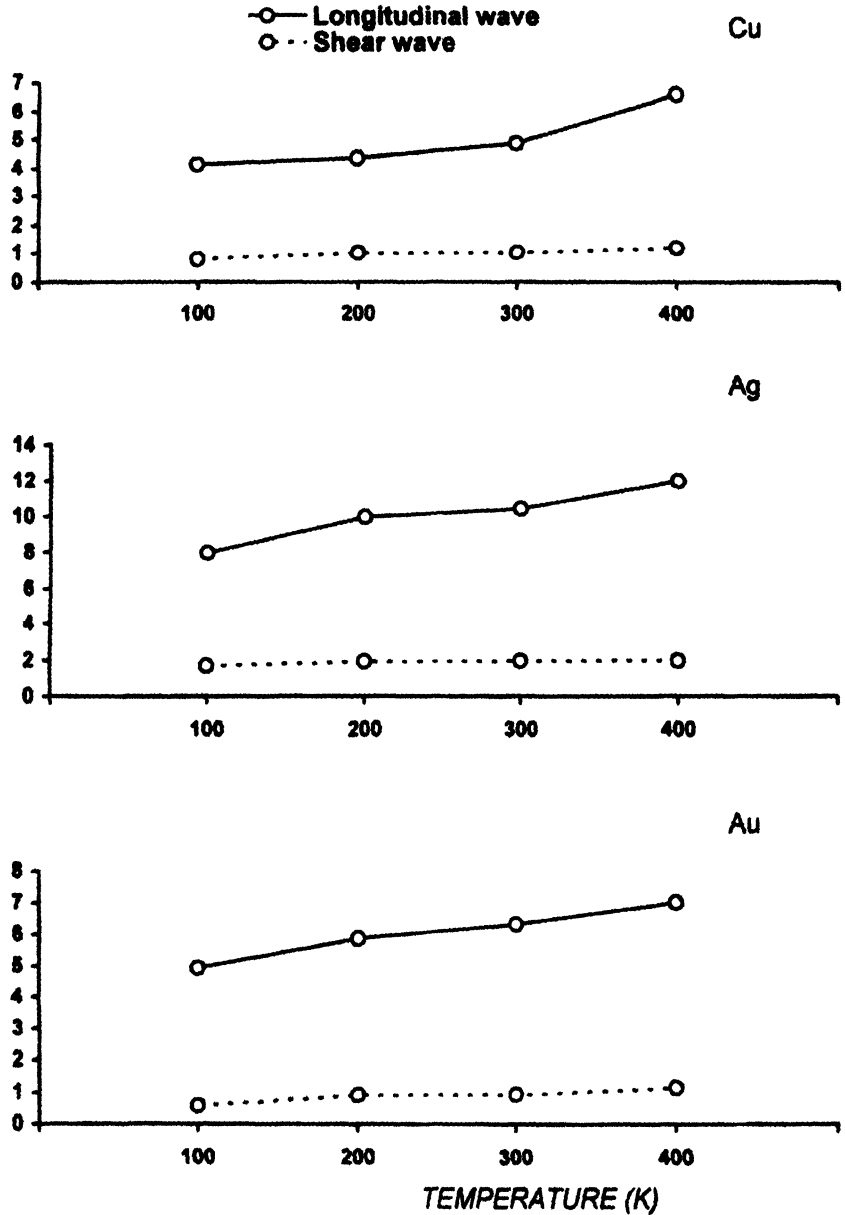


Figure 2. Temperature dependence of nonlinearity constant along  $\langle 100 \rangle$  direction in highly conducting metals.

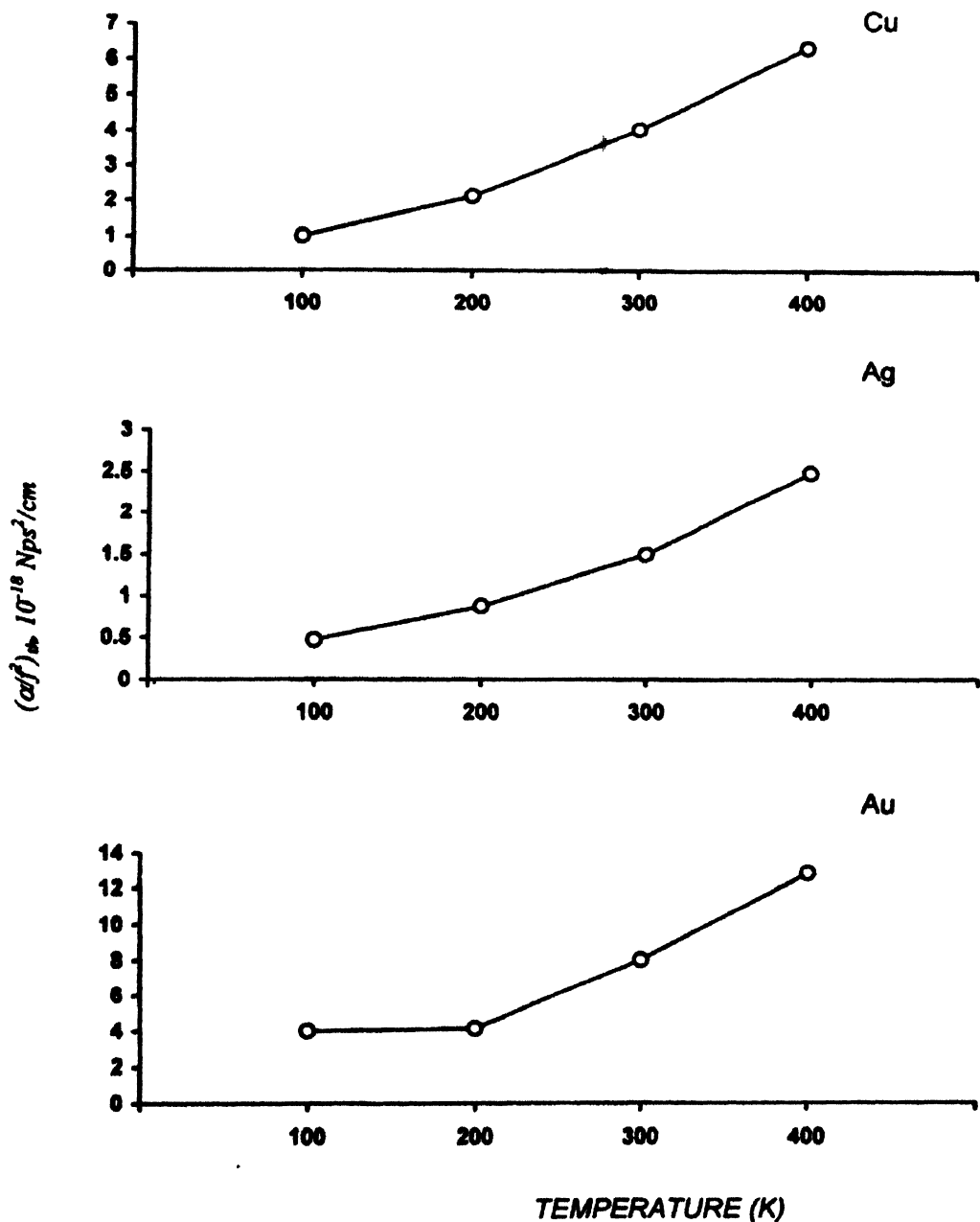
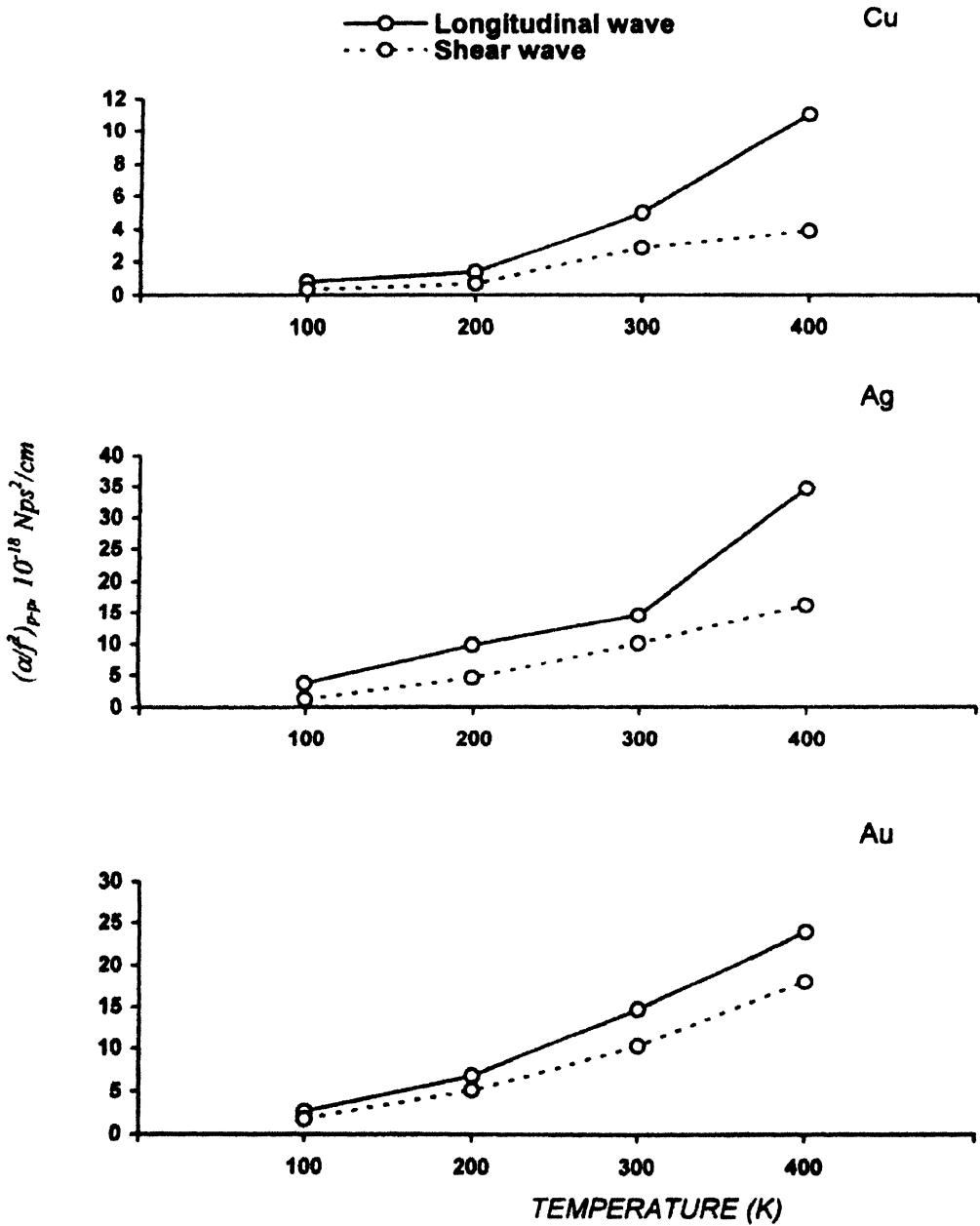


Figure 3. Temperature dependence of thermoelastic loss for longitudinal waves along  $\langle 100 \rangle$  direction in highly conducting metals.



**Figure 4.** Temperature dependence of phonon viscosity loss along  $\langle 100 \rangle$  direction in highly conducting metals.

**Table 5.** Average Gruneisen numbers and nonlinearity constants ratio along <100> direction of propagation in highly conducting metals.

Average Gruneisen numbers & nonlinearity constants ratio	Substances	Temperatures (K)			
		100	200	300	400
$\langle \gamma \rangle_l$	Cu	-0.0203	-0.00332	-0.0279	-0.0187
	Ag	-0.4973	-0.5179	-0.5248	-0.5837
	Au	-0.4001	-0.4318	-0.4589	-0.4818
$\langle \gamma^2 \rangle_l$	Cu	0.4479	0.5176	0.5637	0.7621
	Ag	1.1366	1.2340	1.2362	1.4044
	Au	0.6449	0.7388	0.8199	0.9183
$\langle \gamma \rangle_s$	Cu	0.0809	0.0945	0.1101	0.1274
	Ag	0.2202	0.2214	0.2248	0.2286
	Au	0.1162	0.1247	0.1381	0.1584
$D_l / D_s$	Cu	5.53	5.47	5.11	5.98
	Ag	4.41	4.98	4.96	5.73
	Au	4.50	5.22	5.32	5.23

[29-31], density [29-31] and eq. (8) and (9) and is shown in Figure 1. From eq. (5), the non linearity constants 'D' are obtained taking specific heat [30] and energy [30] of the crystal as a function of temperature (Table 5) and are shown in Figure 2. At last, phonon viscosity and thermoelastic losses,  $(\alpha / f^2)_m$  and  $(\alpha / f^2)_{p-p}$  are calculated from eqs. (6) and (7) and are presented in Figure 3 and 4.

#### 4. Results and discussion

Comparison of calculated and experimental values of thermal relaxation time, Gruneisen numbers, nonlinearity constants, ultrasonic attenuation due to phonon-phonon interaction and thermoelastic loss, with the values for similar substances is the best way to check the validity of present theory.

The value of  $\tau_{th}$  is of the order of  $10^{-11}$ s[33]. From Figure 1, it is clear that at low temperature, its value is very high and decreases as temperature is increased, which is also expected and seen in other types of crystals [32, 33]. After a certain temperature, it achieves, constant value. The expression for temperature variation of thermal relaxation time is

$$\tau_{th} = \tau_0 \exp(-T/\lambda), \tag{10}$$

where  $\tau_0$  and  $\lambda$  are the constants and  $T$  is the absolute temperature.

It can be concluded that non linearity constants increase as temperature increases as shown in Figure 2. This behaviour can be related with atomic mass or atomic number. As atomic number or atomic mass increases, nonlinearity constant will increase in metallic crystals. It is also clear from Table 5 that the ratio of  $D_l/D_s$  lies between 3 and 16 which



is also seen in other types of substances [32, 33].  $D_1$  is greater than  $D_2$  along  $\langle 100 \rangle$  direction of propagation.

In all the three noble metals Cu, Ag and Au,  $(\alpha/f^2)_{p-p}$  is negligible in comparison with p-p interaction. The thermoelastic attenuation due to the thermal conduction between the compressed and expanded parts of acoustic waves increases as temperature is increased and shown in Figure 3.

The values of  $(\alpha/f^2)_{p-p}$  have been calculated using second and third order elastic constants data at 293 K by Tondon *et al* [33]. Attenuation for both longitudinal and shear waves is increasing as the temperature is increased (Figure 4). Ultrasonic attenuation for the shear wave is less than that for the longitudinal wave. The values are in good agreement with the literature [28, 30]. The attenuation varies with temperature as

$$\alpha = \alpha_0 T^n, \quad (11)$$

where  $\alpha$  and  $n$  are constants.

From the above results, one may successfully conclude that ultrasonic attenuation is a fundamental property of the substance.

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