



# Temperature dependent mechanical and thermophysical properties of B-1 phase Ag-Pd alloys

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## Abstract

In present study, we have computed the higher order elastic constants (SOECs and TOECs) of B-1 phase Ag-Pd alloys in the temperature range of 100-500 K with the help of Coulomb and Born-Mayer potential approach. In order to examine the mechanical properties of B-1 phase Ag-Pd alloys, the calculated values of SOECs were utilized to evaluate the Young's modulus, bulk modulus and shear modulus. The SOECs were also used to evaluate the ultrasonic wave velocities for shear and longitudinal modes of propagation along  $\langle 111 \rangle$  orientation in the temperature regime of 100-500 K. Ultrasonic Grüneisen parameters have been computed using Grüneisen number table. We applied the Wiedemann-Franz law to estimate the thermal conductivity of B-1 phase Ag-Pd alloys. Specific heat and thermal energy density have been taken from AIP handbook. The present paper also discusses theoretical evaluation of the thermal relaxation time, anharmonic parameter and ultrasonic attenuation due to phonon-phonon interaction and thermo-elastic relaxation mechanism for Ag-Pd alloys in the temperature range of 100-500 K. The obtained results of present study are in good agreement with properties of available other similar B-1 phase structured materials.

**Keywords:** B-1 phase Ag-Pd alloys, Coulomb and Born-Mayer potential, mechanical properties, thermal properties, ultrasonic attenuation.

## 1. Introduction

Substance having metallic properties of two or more elements is defined as an alloy. In general metals or metalloids are used as key elements for the formation of an alloy. The characteristics of an alloy does not possess similarity with its parent metal or metalloid and this dissimilar characteristic of an alloy increases the applicability/ worthiness of alloy. For a specific application we can manufacture alloy with suitable combination of specific metals or metalloid.

Stainless steel and gold jewellery are

under the category of metal alloy former is manufactured by combining iron, nickel and chromium while later is made up of an alloy of gold and nickel. On the basis of density of metallic alloy, we can use them in various fields. Metallic alloys having high densities are used in the fields which require a high mass-to volume ratio. Aluminium based metal alloys possess low density and are suitable in aerospace field for less fuel consumption. Metal alloys having high fracture toughness are long lasting in nature. In order to understand an alloy system in detail, knowledge about local atomic and

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electronic structure with its energetics is a prerequisite. The metal alloys with discontinuous translational symmetry are more difficult to study, e.g., when there is an interface between the grains. For example, recently with the scanning tunnelling microscope [1] atomic scale observation alloying has become feasible. This has made surface alloying in a two-miscible bimetallic system more fascinating. On account of this, it is very crucial for the accurate estimation of interface due to the reason that the interface regulates the overall feature of thin layered systems, mainly those of magnetic multilayers, which shows large magnetoresistivity [2].

The Ag-Pd system is a binary alloy system well-known for a chaotic metallic solid solution below the melting temperature [3]. Hence Ag-Pd alloy system is persistently used as a perspective material in the study of electronic structure of alloys in general approaches [4-8]. Though some of the experimental studies on Ag-Pd alloys have been surface sensitive, most of the experimental and theoretical investigations available in literature are mainly focused on the bulk properties of the alloys. Lu et al. [9] have reported an electronic structure for particular local configuration of atoms in the substitutionally disordered alloy  $Ag_{1-x}Pd_x$ . This method is based upon the assumption that cluster or impurity atoms are ingrained in a transitionally invariant medium. For different combinations of Ag and Pd, the average site energy in the  $Ag_{0.5}Pd_{0.5}$  alloy rises as the number of like nearest neighbour sites increase. It means that in the bulk alloys, dissimilar near neighbours are energetically preferred to similar near neighbours. Different studies [10-13] have computed the heat of the solution with disordered phase and several stoichiometric compounds utilizing an analytic embedded atom method (EAM) without any adjustable parameter for Ag-Pd. Very few studies so far have been done on the phonon-phonon (p-p) interaction

mechanism and thermoelastic loss mechanism causing ultrasonic attenuation.

In the present chapter metallic alloy  $Ag_{1-x}Pd_x$  (where  $x=1, 2, 3, 4$ ) have been taken for study. Ultrasonic absorption coefficient over frequency due to p-p interaction  $(\alpha/f^2)_{Akh}$  and thermoelastic loss  $(\alpha/f^2)_{th}$  are obtained for longitudinal and shear wave polarised along  $\langle \bar{1}10 \rangle$  direction propagating along  $\langle 111 \rangle$  direction in the temperature range of 100-500K.

## 2. Theory

Using Brügger's definition [14] of second order elastic constants (SOECs) and third order elastic constants (TOECs) have been computed utilizing the nearest neighbour distance and hardness parameter. Temperature dependent SOECs ( $C_{IJ}$ ) and TOECs ( $C_{IJK}$ ) are computed by summing the contribution of vibrational energy part with static elastic constants:

$$C_{IJ} = C_{IJ}^0 + C_{IJ}^{vib} \quad (1)$$

$$C_{IJK} = C_{IJK}^0 + C_{IJK}^{vib} \quad (2)$$

Where superscript 0 indicates SOECs and TOECs at 0K and superscript Vib. stands for contribution of vibrational energy part of SOECs and TOECs due to high temperature of the material.

For B-1 phase materials, Born's mechanical stability criterion is satisfied as

$$B = \left( \frac{C_{11} + 2C_{12}}{3} \right) > 0;$$

$$C_S = \left( \frac{C_{11} - C_{12}}{2} \right) > 0; \quad C_{44} > 0$$

Where  $B$  = bulk modulus and  $C_S$  = tetragonal shear modulus.

Adopting the method mentioned in the literature [15-16], the Young's modulus

(Y), shear modulus (G) and bulk modulus (B) has been estimated theoretically.

In order to evaluate the ultrasonic attenuation at higher temperatures (in vicinity of room temperature) in solids, Mason-Bateman[17] theory has been used. In this theory, elastic constants are directly correlated to anharmonic parameter 'D' in the computation of ultrasonic absorption coefficient ( $\alpha$ ) hence this theory is more reliable to investigate the anharmonicity of the crystals. The magnitude of thermal relaxation time[17] for shear wave is half that for longitudinal wave and is related to specific heat per unit volume ( $C_V$ ) and thermal conductivity (K) as follows:

$$\tau_{th} = \tau_{shear} = \frac{1}{2} \tau_{long} = \frac{3K}{C_V \bar{V}^2} \quad (3)$$

Where  $\bar{V}$  is the Debye average velocity of the ultrasonic wave and given as

$$3 / \bar{V}^3 = 1 / V_l^3 + 2 / V_s^3 \quad (4)$$

Thermoelastic loss[17] is given by the expression

$$(\alpha / f^2)_{th} = \frac{4\pi^2 \langle \gamma_i^j \rangle^2 KT}{2\rho V_{long}^5} \quad (5)$$

Where  $\gamma_i^j$  is the Grüneisen parameters. Ultrasonic Grüneisen parameters (UGPs), which describe the relative strain dependence of elastic wave velocity and provide the thermal and the mechanical characteristics of materials. UGPs are used to investigate the anharmonicity of a crystal[18]. The lattice-specific heat at high temperature, thermal conductivity, thermal expansion, temperature variation have been characterised by UGPs. UGPs define the phonon distribution to a variety of anharmonic characteristics like specific heat, thermal properties and so on. The expressions to compute UGPs have been given in literature.[18,19]

The ultrasonic absorption coefficient over frequency square  $(\alpha/f^2)_{Akh}$  is given by  $(\omega\tau \ll 1)$ [19]

$$(\alpha / f^2)_{Akh} = \frac{4\pi^2 \tau E_o (D/3)}{2\rho V^3} \quad (6)$$

To evaluate  $(\alpha/f^2)_{Akh}$ , we have evaluated 'D' which quantify the transformation of acoustic energy into thermal energy and is formulated as:

$$D = 9 \langle \gamma_i^j \rangle^2 > - \frac{3 \langle \gamma_i^j \rangle^2 KT}{E_o} \quad (7)$$

$\langle \gamma_i^j \rangle$  are the average Grüneisen numbers which are connected with SOECs and TOECs and computed via Mason's table[17] and presented in Table 6.

By determining  $D_{long}$  and  $D_{Shear}$  for longitudinal and shear wave;  $(\alpha/f^2)_{Akh, long}$  and  $(\alpha/f^2)_{Akh, shear}$  can be evaluated.

### 3.Results and Discussion

The SOECs and TOECs have been computed starting with nearest neighbour distance[20]  $Ag_{99}Pd_1=2.039\text{\AA}$ ,  $Ag_{98}Pd_2=2.038\text{\AA}$ ,  $Ag_{97}Pd_3=2.037\text{\AA}$  and  $Ag_{96}Pd_4=2.036\text{\AA}$  and hardness parameter[21]  $b=0.315\text{\AA}$  taking equal for all alloys. For cubic crystal, hardness parameter in the Born-Mayer potential  $\phi(r_0)=A \exp(-r_0/b)$  is calculated using concept of maxima-minima in the expression given as follows[22]

$$-(e^2 / r_0) S_3^{(1)} - (2r_0 / b) \phi(r_0) - (4\sqrt{2}r_0 / b) \phi(\sqrt{2}r_0) + (\eta\omega_0 / 4) G_1 Cothx = 0$$

Some specific values of b which satisfies above expression as well as minimizes  $\sum(C_{ij}^{cal.} - C_{ij}^{exp.})^2$  are picked up as the most probable one. Approximate value of b has been taken for other compounds mentioned in the literature[22]. Ghate[23] used two values of hardness parameter for

rock salt crystals[21]. The value of 'b' is temperature independent and practical value of b is  $0.315 \times 10^{-10}$  m which is almost same for all the four compounds. The

obtained values of SOECs and TOECs along with Y, B and G have been presented in Tables 1-4.

**Table 1:** SOECs, TOECs, and Y,B, G in  $10^{11}$  Dyne/cm<sup>2</sup> of Ag<sub>99</sub>Pd<sub>1</sub> at temperature range of 100-500K.

SOEC & TOEC	100K	200K	300K	400K	500K
C <sub>11</sub>	8.105	8.104	8.129	8.202	8.315
C <sub>12</sub>	6.071	6.055	5.998	5.919	5.833
C <sub>44</sub>	6.369	6.371	6.377	6.389	6.404
C <sub>111</sub>	-99.053	-98.975	-98.774	-98.678	-98.765
C <sub>112</sub>	-24.587	-24.605	-24.544	-24.389	-24.189
C <sub>123</sub>	8.504	8.384	8.100	7.776	7.447
C <sub>144</sub>	9.189	9.198	9.226	9.267	9.313
C <sub>166</sub>	-25.699	-25.698	-25.703	-25.725	-25.761
C <sub>456</sub>	9.054	9.054	9.054	9.054	9.054
Y	8.552	8.569	8.657	8.820	9.027
B	6.749	6.738	6.708	6.68	6.660
G	3.139	3.147	3.191	3.270	3.3712

**Table 2:** SOECs, TOECs, and Y, B, G in  $10^{11}$  Dyne/cm<sup>2</sup> of Ag<sub>98</sub>Pd<sub>2</sub> at temperature range 100-500K.

SOEC & TOEC	100K	200K	300K	400K	500K
C <sub>11</sub>	7.667	7.679	7.752	7.879	8.038
C <sub>12</sub>	6.133	6.091	6.013	5.925	5.836
C <sub>44</sub>	6.347	6.351	6.362	6.378	6.397
C <sub>111</sub>	-96.539	-96.373	-96.282	-96.439	-96.790
C <sub>112</sub>	-24.804	-24.783	-24.629	-24.419	-24.197
C <sub>123</sub>	8.666	8.436	8.112	7.784	7.457
C <sub>144</sub>	9.169	9.189	9.230	9.278	9.327
C <sub>166</sub>	-25.589	-25.591	-25.613	-25.654	-25.708
C <sub>456</sub>	9.071	9.071	9.071	9.071	9.071
Y	7.959	8.0242	8.205	8.454	8.730
B	6.644	6.620	6.592	6.576	6.570
G	2.869	2.899	2.984	3.101	3.233

**Table 3: SOECs, TOECs, and Y, B, G in  $10^{11}$  Dyne/cm<sup>2</sup> of Ag<sub>97</sub>Pd<sub>3</sub> at temperature range 100-500K.**

SOEC	100K	200K	300K	400K	500K
C <sub>11</sub>	7.474	7.504	7.609	7.761	7.939
C <sub>12</sub>	6.165	6.108	6.023	5.934	5.844
C <sub>44</sub>	6.344	6.351	6.365	6.383	6.404
C <sub>111</sub>	-95.407	-95.229	-95.275	-95.584	-96.059
C <sub>112</sub>	-24.930	-24.863	-24.672	-24.451	-24.225
C <sub>123</sub>	8.733	8.454	8.126	7.799	7.474
C <sub>144</sub>	9.171	9.199	9.245	9.294	9.344
C <sub>166</sub>	-25.569	-25.577	-25.610	-25.661	-25.722
C <sub>456</sub>	9.089	9.089	9.089	9.089	9.089
Y	7.678	7.789	8.027	8.316	8.622
B	6.601	6.573	6.551	6.543	6.542
G	2.742	2.793	2.903	3.037	3.182

**Table 4: SOECs, TOECs, and Y, B, G in  $10^{11}$  Dyne/cm<sup>2</sup> of Ag<sub>96</sub>Pd<sub>4</sub> at temperature range 100-500K.**

SOEC	100K	200K	300K	400K	500K
C <sub>11</sub>	7.360	7.407	7.533	7.701	7.889
C <sub>12</sub>	6.188	6.121	6.034	5.944	5.854
C <sub>44</sub>	6.348	6.357	6.373	6.392	6.414
C <sub>111</sub>	-94.716	-94.563	-94.717	-95.121	-95.667
C <sub>112</sub>	-25.025	-24.921	-24.714	-24.489	-24.263
C <sub>123</sub>	8.771	8.469	8.142	7.819	7.492
C <sub>144</sub>	9.180	9.215	9.262	9.312	9.362
C <sub>166</sub>	-25.579	-25.593	-25.634	-25.691	-25.756
C <sub>456</sub>	9.107	9.107	9.107	9.107	9.107
Y	7.505	7.656	7.930	8.244	8.567
B	6.578	6.549	6.533	6.529	6.532
G	2.665	2.733	2.858	3.003	3.155

The computed values of ultrasonic velocities *i.e.*, for longitudinal and shear waves have been computed with SOECs ( $C_{11}$  and  $C_{44}$ ) and density of the alloys. These values of ultrasonic velocities have been used to compute Debye average velocity. These values are tabulated in Table 5. The ultrasonic velocities are increasing with temperature due to the values of SOECs ( $C_{11}$  and  $C_{44}$ ).

The specific heat( $C_v$ ), energy density ( $E_0$ ) and density  $\rho$  of the alloys are taken from the literature[20].The electrical resistivity data is taken from the literature[24]. The thermal conductivity for the different given compositions of the alloys are calculated by

applying Wiedemann-Franz law  $\frac{K}{\sigma} = L_0 T$ ,

Where  $L_0$  is the Lorentznumber ( $L_0 = \frac{\pi^2}{3} (\frac{k_B}{e})^2$ ). Where  $k_B$  is Boltzmann constant and  $e$  is the electronic charge and  $\sigma = \frac{1}{R}$  where  $R$  is the electrical resistivity.

The computed values of specific heat ( $C_v$ ), thermal conductivity ( $K$ ), density ( $\rho$ ) and internal energy density ( $E_0$ ) of the alloy are presented in Table 5.

**Table 5:**  $K$  in  $10^7$  erg/cm s K, density ( $\rho$ ) in g/cc,  $C_v$  in  $10^7$  erg/cc K, thermal energy density ( $E_0$ ) in  $10^8$  erg/cc ultrasonic velocities ( $V_l$  for longitudinal wave,  $V_s$  for shear wave and  $\bar{V}$  for Debye average velocity in  $10^5$  cm/s and  $\tau_{th}$  in  $10^{-11}$  s for metallic alloy.

Material	Temp.(K)	K	$\rho$	$C_v$	$E_0$	$V_l$	$V_s$	$\bar{V}$	$\tau_{th}$
Ag <sub>99</sub> Pd <sub>1</sub>	100	4.900	10.52	1.900	9.439	2.776	2.461	2.518	12.202
	200	5.440	10.45	2.280	30.969	2.785	2.469	2.527	11.212
	300	5.650	10.39	2.330	53.747	2.797	2.477	2.536	11.313
	400	5.765	10.32	2.350	76.804	2.819	2.488	2.549	11.327
	500	6.125	10.28	2.353	99.906	2.844	2.496	2.561	11.909
Ag <sub>98</sub> Pd <sub>2</sub>	100	2.227	10.53	1.902	9.449	2.698	2.455	2.495	5.642
	200	3.266	10.48	2.289	31.061	2.707	2.461	2.502	6.867
	300	3.868	10.41	2.339	53.855	2.729	2.472	2.515	7.841
	400	4.455	10.34	2.355	77.105	2.760	2.484	2.532	8.854
	500	4.712	10.25	2.359	100.012	2.800	2.498	2.552	9.199
Ag <sub>97</sub> Pd <sub>3</sub>	100	1.633	10.55	1.906	9.469	2.662	2.452	2.484	4.167
	200	2.578	10.49	2.291	30.965	2.675	2.460	2.493	5.432
	300	3.196	10.40	2.337	53.813	2.705	2.474	2.511	6.509
	400	3.769	10.33	2.353	76.900	2.741	2.486	2.529	7.516
	500	4.083	10.28	2.354	99.632	2.779	2.496	2.545	8.031
Ag <sub>96</sub> Pd <sub>4</sub>	100	1.167	10.56	1.908	9.479	2.640	2.452	2.478	2.989
	200	2.042	10.49	2.268	30.837	2.657	2.462	2.489	4.359
	300	2.625	10.42	2.342	53.715	2.689	2.473	2.506	5.355
	400	3.161	10.35	2.358	76.749	2.728	2.485	2.525	6.309
	500	3.500	10.29	2.364	99.629	2.769	2.497	2.543	6.866

The thermal relaxation time ( $\tau_{th}$ ) are evaluated taking thermal conductivity of the

requisite composition of the alloys with the help of Eq. (3). The thermoelastic loss

$(\alpha/f^2)_{th}$ , and ultrasonic absorption coefficient over frequency square  $(\alpha/f^2)_{Akh}$ , due to phonon-phonon interactions are evaluated at the temperature range 100-500K using Eq. (5) and (6).

Till now, the experimental values of the SOECs and TOECs of the Ag-Pd alloys have been not reported hence we compared our outcomes with other alloy Cu-Ni[25]. The order of values of SOECs and TOECs is similar ( $\approx 10^{11}$  dyne/cm<sup>2</sup>). The present investigation may be very interesting with reference to these results. TOECs play vital role to study the anharmonicity of the crystal and reveals the different intrinsic characteristics of the crystals. One may expect the variation in the values of all the six constants according to the variation of composition of Ag and Pd. It is clear from

Table 1-4 that in the chosen alloys, the values of  $C_{112}$ ,  $C_{123}$  and  $C_{456}$  are increasing with increase in percentage of Pd whereas values of  $C_{111}$ ,  $C_{166}$  are decreasing with addition of Pd. According to the variation in TOECs, the change in values of 'D' are also observed. It is evident from the Table 5 that the thermal relaxation time ( $\tau_{th}$ ) decreases for all the alloys as the percentage of palladium increases. The magnitude of relaxation time is  $10^{-11}$ s, which is similar with other metallic alloy[25]. For  $Ag_{99}Pd_1$ ,  $\tau_{th}$  decreases with increase in temperature whereas reversal in nature of  $\tau_{th}$  is found with increase in palladium concentration. All the calculated values of the non-linearity parameter 'D' are presented in Table 6.

**Table 6:** Average Grüneisen numbers  $\langle \gamma_i^j \rangle_1$  for longitudinal wave, average square Grüneisen numbers  $\langle (\gamma_i^j)^2 \rangle_1$  for longitudinal wave, average square Grüneisen numbers  $\langle (\gamma_i^j)^2 \rangle_s$  for shear wave polarised along  $\langle \bar{1} 10 \rangle$  direction,  $D_l$  and  $D_s$  for longitudinal and shear wave polarised along  $\langle \bar{1} 10 \rangle$  direction all along  $\langle 111 \rangle$  direction of the metallic alloy.

Material	Temp.(K)	$\langle \gamma_i^j \rangle_1$	$\langle (\gamma_i^j)^2 \rangle_1$	$\langle (\gamma_i^j)^2 \rangle_s$	$D_l$	$D_s$
Ag <sub>99</sub> Pd	100	-0.696	3.113	0.984	25.096	8.856
	200	-0.692	3.075	0.981	25.562	8.825
	300	-0.676	2.910	0.965	24.407	8.685
	400	-0.651	2.659	0.939	22.384	8.459
	500	-0.622	2.397	0.912	20.209	8.205
Ag <sub>98</sub> Pd	100	-0.797	4.404	1.106	35.799	9.950
	200	-0.781	4.175	1.087	34.884	9.779
	300	-0.741	3.666	1.041	30.849	9.371
	400	-0.696	3.141	0.991	26.491	8.921
	500	-0.653	2.703	0.946	22.815	8.517
Ag <sub>97</sub> Pd	100	-0.864	5.457	1.202	44.607	10.816
	200	-0.831	4.931	1.158	41.316	10.419
	300	-0.773	4.098	1.084	34.545	9.753
	400	-0.716	3.382	1.016	28.558	9.144
	500	-0.666	2.844	0.961	24.024	8.653
Ag <sub>96</sub> Pd	100	-0.915	6.388	1.288	52.438	11.588
	200	-0.865	5.510	1.213	46.291	10.917
	300	-0.793	4.395	1.113	37.086	10.016
	400	-0.728	3.539	1.032	29.896	9.287

500	-0.674	2.933	0.971	24.782	8.736
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The ratio of  $D_l$  and  $D_s$  for shear wave polarised along  $\langle \bar{1}10 \rangle$  in  $\langle 111 \rangle$  direction is approximately 5-23. This is very much similar to other metallic crystals and metallic alloys [22,23]. The evaluated ultrasonic absorption coefficient  $(\alpha/f^2)$  due to p-p interaction  $[(\alpha/f^2)_{Akh.long}$  for

longitudinal wave and  $(\alpha/f^2)_{Akh.shear}^*$  for shear wave] and thermoelastic loss  $(\alpha/f^2)_{th}$  are presented in Table 7 along  $\langle 111 \rangle$  direction of propagation for longitudinal and shear wave polarised along  $\langle \bar{1}10 \rangle$  direction respectively.

**Table 7:**  $(\alpha/f^2)_{Akh.long}$  and  $(\alpha/f^2)_{Akh.shear}^*$  and thermoelastic loss  $(\alpha/f^2)_{th}$  in the metallic alloy at the temperature range 100-500K along  $\langle 111 \rangle$  direction in  $10^{-16}$  Nps<sup>2</sup>/cm.

Material	Temp.(K)	$(\alpha/f^2)_{th}$	$(\alpha/f^2)_{Akh.long}$	$(\alpha/f^2)_{Akh.shear}^*$
Ag <sub>99</sub> Pd <sub>1</sub>	100	0.540	1.689	0.428
	200	1.159	5.170	1.280
	300	1.591	8.579	2.197
	400	1.751	11.071	3.043
	500	1.814	13.367	4.015
Ag <sub>98</sub> Pd <sub>2</sub>	100	0.565	1.213	0.224
	200	1.474	4.685	0.873
	300	1.952	8.095	1.654
	400	2.091	10.932	2.527
	500	1.922	12.259	3.226
Ag <sub>97</sub> Pd <sub>3</sub>	100	0.680	1.163	0.180
	200	1.722	4.552	0.737
	300	2.109	7.729	1.426
	400	2.128	10.199	2.189
	500	1.911	11.452	2.848
Ag <sub>96</sub> Pd <sub>4</sub>	100	0.693	1.005	0.139
	200	1.759	4.156	0.616
	300	2.049	6.924	1.202
	400	1.998	9.060	1.861
	500	1.773	10.200	2.453



From Table 7 it is obvious that the thermoelastic loss  $(\alpha/f^2)_{th}$  for  $Ag_{99}Pd_1$  first increases with increase in temperature. After the temperature 450K it saturates. This is because of the variations in Grüneisen parameters of the alloys. Maximum of attenuation  $(\alpha/f^2)_{th}$  is being shifted towards higher value with the higher concentration of Pd in the alloy. Thus, the quantitative behaviour of ultrasonic attenuation with the temperatures in the alloys depends upon the concentration of the components of the alloy. The observed behaviour will be characteristic because the attenuation is well connected to the microstructural and physical properties of the alloys. There is a regular variation of  $(\alpha/f^2)_{Akh}$  [both for longitudinal and shear wave] from 1% of Pd to 4% of Pd. This value increases with increase in temperature. Here, the variation of  $(\alpha/f^2)_{Akh}$  is more affected by thermal conductivity value rather than other parameters of the alloys. The values of  $(\alpha/f^2)_{Akh}$  for longitudinal wave is greater than that for shear wave along all the directions with the increase in temperature. This is because of the values of anharmonic parameter 'D' for that direction in the temperature range. Despite the fact that experimental values of attenuation are not available for comparison, it is justified that our values are right, keeping in view the magnitude of attenuation evaluated in the present investigation. Generally, the values of attenuation obtained in the present work are comparable with the values available for the other metals [22,23]. One may conclude that the quantitative behaviour of alloys is in general similar to that of metallic crystals [22,23]. However, the alloys show some characteristic attenuation values at particular temperatures as discussed.

Also, the method used for evaluation of ultrasonic attenuation in metals can be used successfully in alloys. Ultrasonic testing which is a versatile non-destructive testing for the detection of surface or volume defects, such as laps, seams, voids, cracks etc. in alloys are very much useful in oil engineering and material sciences.

#### 4. Conclusions

With the help of lattice parameter and hardness parameter and following the Coulomb and Born-Mayer potential model, the temperature dependent numerical values of SOECs and TOECs have been obtained. The obtained values have been compared with other B1 structured materials existing in the literature. We find that the compared values display similar order of magnitude which asserts the method followed by us for the evaluation of temperature dependent SOECs and TOECs. We observe that with increase in temperature, Y and G increase in small amount while B decreases slightly. Small positive variation has been displayed by Longitudinal and shear wave velocities in the chosen alloys with the increment in temperature. The order of relaxation time is  $10^{-11}$  s, which confirms the metallic nature of the selected alloys. When the temperature is increased, the values of anharmonic parameter show decremental nature for both longitudinal and shear modes of vibration. The attenuation caused via phonon-phonon interaction dominates over the attenuation caused by thermal relaxation process.

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