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Conclusive Research Design and Development of the Effect of Linear Deformation on Some Debye Properties of Metals

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Abstractin This Work, Debye Temperature And Debye Frequency Of Metals Were Computed And Studied Using Quantum Einstein Theory. The Electron Density Parameters Of Strained Metals Is Obtained And Used In The Computation.. The Results Obtained Revealed That There Is Agreement Between The Computed And Experimental Values Of Debye Temperature And Debye Frequency. This Shows That The Model Can Be Used To Study Debye Properties Of Metals. The Debye Temperature And Debye Frequency Obtained Are More Concentrated In The High Density Limit. **This Revealed That *Debye Temperature And* Debye Frequency Of Metals Depend On The Electronic Concentration. Also, The Experimental Value Of *Debye Temperature And Debye Frequency Is Higher Than The Computed Value, This Is Because Of Some Factor Which Debye Temperature And Debye Frequency Relied On That The Theory Failed To Account For.* Debye Temperature And Debye Frequency Of Metals Reduces As Strain Increase. This Shows That As Strain Increase, Space Between Lattice Atom Increase Which Reduces Strength Of Electron Interaction And There-By Forces Debye Temperature, Debye Frequency To Decrease As Deformation Increase. This Behavior Of Metals Reveal That Debye Temperature And Debye Frequency Is Greatly Affected By Deformation.**

Keywords: Deformation, Einstein model, Debye temperature, Debye frequency, poison ratio. Electron density parameter

I. INTRODUCTION

Solid consists of a sufficiently large collection of atoms that exhibit the characteristic behavior of bulk material, the atom may lose some of its tightly bound electrons leaving the core electrons, such entity is known as ions (Rogalski and Palmer, 2000). At a finite temperature, the atoms in a crystalline lattice vibrate about their equilibrium positions with amplitude that is temperature dependent, these vibrations can be explained in terms of collective modes of motion of the ions. When atom vibrates, the force on atoms changes causing them to vibrate (Efthimios, 2003). Crystal lattice dynamics can be discussed in the frame of the adiabatic approximation by solving Hamiltonian operator for the motion of the ions about their equilibrium position which defines the lattice spatial distribution. Lattice vibrations can be described in terms of waves propagating along a linear chain, such that the amplitude of the vibration for the atom is equal in the Debye approximation, a linear lattice can sustain long wavelength elastic waves which propagate without dispersion (Rogalski and Palmer, 2000). Debye model of solid treats the frequency spectrum as linearly dependent on the wave-vectors for all modes. For a realistic computation, the actual frequency spectrum is included to give a density of states with features that relied on the structure of solid (Efthimios, 2003). The Debye model is an isotropic continuum where motion of an atom influences its neighbor's motion. Atomic vibrations have complete spectrum of frequencies which vary in a continuous fashion, the medium is dispersion-less and the velocity of sound is independent of the frequency and the number of standing sound waves that can be fitted in the solid with frequencies in the range between vibrating mode to determines the spectrum which is characterized by a cut-off frequency known as Debye frequency (Kachava, 1992). Deformation is when metals undergo compressive force, torsion force or tensile force and the shape or size becomes different. Because of the anisotropy of a crystal, the atoms of any crystal can be deformed in a variety of ways that can be decomposed into three types of independent deformations viz, uniform compression associated with the bulk modulus or compressibility and two shears in both of which the volume is unchanged (Animalu, 1977). Mathematically, any lattice deformation can be characterized by a second-rank tensor η_{ij}, called a strain tensor which has three independent components in a system with cubic symmetry (Animalu, 1977).Consequently, a lot of success have been recorded in the study of deformed properties of metals theoretically and experimentally. Kiejna and Pogosov (1999) investigated experimentally the effect of deformation on electronic properties of metals based on Kelvin method. The result obtained shows that contact potential difference of the metals increase/decrease when compressed/tensed. Pogosov and Shtepa, (2006), studied surface stress and contact potential difference of elastically strained metals based on structureless pseudopotential formalism. The results obtained were in agreement with experimental results.

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Adeshakin and Osiele (2012) theoretically studied the surface energy and surface stress of strained metals using structureless pseudopotential model.
The results obtained revealed that deformation causes a reduction of surface energy, some metals have tensile stress on their surfaces while some have compressive stress on their surfaces. Surface stress of some metals decreases as deformation increases while some increases. Adeshakin et al. (2012) applied structureless pseudopotential to study correlation, binding and cohesive energy of metals. The result obtained is in agreement with experimental values. The results obtained show that deformation decreases the binding energy of metals but does not significantly affect cohesive energy of metals. Adeshakin *et. al* (2015) computed the electron density parameter, Fermi energy, Fermi wave vector and chemical potential of strained metals using structureless pseudopotential. The results obtained revealed that deformation affect electron density parameter, Fermi wave vector, Fermi energy and chemical potential of metals. Adesakin, (2018), *computed electronic heat capacity of metals based on Einstein model formalism. There is agreement between the computed and experimental values which shows the validity of Einstein model in studying the electronic heat capacity of metals.* The electronic heat capacity of all the metals increases as deformation (strain) increases. This is because as the collision between the interacting electron increases the electron thermal excitation also increases and there-by result in the increase in the electronic heat capacity as deformation increases.

In this work, Einstein model is extended to study Debye temperature and Debye frequency of metal. The metals were chosen based on experimental data available and physical constants required for computation.

II. THEORETICAL EXPRESSION FOR DEBYE PROPERTIES OF METALS

The internal energy per unit volume of quantum mechanical calculation in terms of phonons is

$$\frac{E}{\Omega}=\frac{1}{\Omega}\frac{\sum_s E_s exp(-\beta E_s)}{\sum_s exp(-\beta E_s)}$$

(1)

Where, E_s is the energy corresponding to a particular state of the system which involves a number of excited phonons. The total energy due to the phonon excitations is given by

$$E_s=\sum_{k,l}\left(n_{ks}^l+\frac{1}{2}\right)\hbar\omega_k^l$$

(2)

l is the index and k is the wave-vector. In classical discussion, the total energy is

$$\frac{E}{\Omega}=-\frac{1}{\Omega}\frac{\partial}{\partial\beta}ln\left(\sum_s exp-\beta E_s\right)$$

(3)

using mathematical trick to express this in a more convenient form. Consider the expression

$$\sum_s exp-\beta E_s=\sum_s exp\left[-\sum_{k,l}\left(n_{ks}^l+\frac{1}{2}\right)\hbar\omega_k^l\beta\right]$$

(4)

Which involves a sum of all exponentials containing terms $\left(n_{ks}^l+\frac{1}{2}\right)\hbar\omega_k^l\beta$ with all possible non-negative integer values of n_{ks}^l. The expression

$$\prod_{k,l}\sum_{n=0}^{\infty}exp-\beta\left(n+\frac{1}{2}\right)\hbar\omega_k^l=\left(exp-\beta\hbar\frac{1}{2}\omega_{k_1}^{l_1}+exp-\beta\hbar\frac{3}{2}\omega_{k_1}^{l_1}+\cdots\right)\left(exp-\beta\hbar\frac{1}{2}\omega_{k_2}^{l_2}+exp-\beta\hbar\frac{3}{2}\omega_{k_2}^{l_2}+\cdots\right)$$

(5)

Substituting equation (5) into equation (3) gives the summation geometric series as

$$\sum_{n=0}^{\infty}exp-\beta\left(n+\frac{1}{2}\right)\hbar\omega_k^l=\frac{exp-\beta\hbar^{\omega_k^l/2}}{1-exp-\beta\hbar\omega_k^l}$$

(6)

The total internal energy per unit volume is

$$\frac{E}{\Omega}=-\frac{1}{\Omega}\frac{\partial}{\partial\beta}ln\left[\prod_{k,l}\frac{exp-\beta\hbar^{\omega_k^l/2}}{1-exp-\beta\hbar\omega_k^l}\right]=\frac{1}{\Omega}\sum_{k,l}\hbar\omega_k^l\left(\bar{n}_k^l+\frac{1}{2}\right)$$

(7)

Where $\bar{n}_k^l(T)=\frac{1}{exp\beta\hbar\omega_k^l}$

(8)

The quantity $\bar{n}_k^l(T)$ represents the average occupation of the phonon state with frequency ω_k^l at temperature T. From equation (7), the specific heat per unit volume is

$$C_v=\frac{\partial}{\partial T}\left[\frac{E}{\Omega}\right]=\frac{1}{\Omega}\sum_{K,L}\hbar\omega_k^l\frac{\partial}{\partial T}\bar{n}_k^l(T)$$

(9)

Turning the summation into an integral, the specific heat in equation (9) become

$$C_v=\frac{\partial}{\partial T}\sum_i\int\frac{dk}{(2\pi)^3}\frac{\hbar v_k^l k}{exp\hbar v_k^l k\beta-1}$$

(10)

Differentiating equation (10), the heat capacity can be express as

$$C_v=\int_0^{v_{max}}k_B\left(\frac{\hbar\omega}{k_BT}\right)^2\frac{exp\left(^{\hbar\omega}/_{k_BT}\right)}{\left(exp\left(^{\hbar\omega}/_{k_BT}\right)-1\right)^2}N(\omega)d\omega$$

(11)

$N(\omega)d\omega$ is the number of oscillators with frequencies range, v_{max} is the Debye frequency which is the highest frequency of any normal mode.
To be able to compare equation (11) with experimental value of heat capacity, consider the three-dimensional case where a system of N ions has 3N degree of freedom (N-ions=3N) independent quantum oscillators and the normalization condition is

$$\int_0^{v_{max}}N(\omega)d\omega=3N \qquad (12)$$

Since every lattice point is associated with one longitudinal mode and two transverse modes with phase velocities v_l and v_t respectively for any given frequency v we have

$$N(\omega)=\frac{V\omega^2}{2\pi^2}\left(\frac{1}{v_l^3}+\frac{2}{v_t^3}\right)=\frac{3V}{2\pi^2v^3}\omega^2$$

(13)

v is the mean phase velocity. Putting equation (13) into equation (12)

$$\int_0^{\nu_{max}} \frac{V\omega^2}{2\pi^2}\left(\frac{1}{{v_l}^3}+\frac{2}{{v_t}^3}\right) d\omega = \int_0^{\nu_{max}} \frac{3V}{2\pi^2 v^3}\,\omega^2 d\omega$$

(14)

$$\frac{V}{2\pi^2}\left(\frac{1}{{v_l}^3}+\frac{2}{{v_t}^3}\right)\int_0^{\nu_{max}} \omega^2 d\omega = \frac{3V}{2\pi^2 v^3}\int_0^{\nu_{max}} \omega^2 d\omega$$

(15)

$$\frac{V}{2\pi^2}\left(\frac{1}{{v_l}^3}+\frac{2}{{v_t}^3}\right)\left[\frac{\omega^3}{3}\right]_0^{\nu_{max}} = \frac{3V}{2\pi^2 v^3}\left[\frac{\omega^3}{3}\right]_0^{\nu_{max}}$$

(16)

$$\frac{V}{2\pi^2}\left(\frac{1}{{v_l}^3}+\frac{2}{{v_t}^3}\right)\left(\frac{\nu_{max}^3}{3}\right) = \frac{3V}{2\pi^2 v^3}\left(\frac{\nu_{max}^3}{3}\right)$$

(17)

Recall that both side of equation (17) is equal to 3N

$$\frac{V}{2\pi^2}\left(\frac{1}{{v_l}^3}+\frac{2}{{v_t}^3}\right)\left(\frac{\nu_{max}^3}{3}\right) = 3N \qquad (18)$$

then

$$\frac{V}{2\pi^2}\left(\frac{1}{{v_l}^3}+\frac{2}{{v_t}^3}\right) = \frac{9N}{\nu_{max}^3}$$

(19)

and

$$\frac{3V}{2\pi^2 v^3}\left(\frac{\nu_{max}^3}{3}\right) = 3N$$

(20)

$$\frac{3V}{2\pi^2 v^3}=\frac{9N}{\nu_{max}^3} \qquad (21)$$

therefore

$$\frac{V}{2\pi^2}\left(\frac{1}{{v_l}^3}+\frac{2}{{v_t}^3}\right) = \frac{3V}{2\pi^2 v^3} = \frac{9N}{\nu_{max}^3} \qquad (22)$$

Since equation (19) and equation (21) is the same, the Debye frequency or cut-off frequency ν_{max} is obtained using equation (21) as

$$\nu_{max} = v\left(6\pi^2\frac{N}{V}\right)^{1/3} \qquad (23)$$

Substituting equation (19) and equation (21) into equation (13) we have

$$N(\omega) = \frac{9N}{\nu_{max}^3}\,\omega^2$$

(24)

Using the frequency distribution function, the lattice heat capacity in equation (11) can be written as

$$C_v = \frac{9Nk_B}{\nu_{max}^3}\int_0^{\nu_{max}}\left(\frac{\hbar\omega}{k_BT}\right)^2 \frac{\omega^2 exp\left(\hbar\omega/_{k_BT}\right)}{\left(exp\left(\hbar\omega/_{k_BT}\right)-1\right)^2} d\omega$$

(25)

When $x = \hbar\omega/_{k_BT}$ then

$$C_v = 9Nk_B\left(\frac{T}{\theta_D}\right)^3\int_0^{\theta_D/_T}\frac{x^4\exp(x)}{(\exp(x)-1)^2}dx$$

(26)

By integrating equation (26), the Debye temperature θ_D is obtained as

$$\theta_D = \frac{\hbar\nu_{max}}{k_B} = \frac{\hbar v}{k_B}\left(6\pi^2\frac{N}{V}\right)^{1/3} \qquad (27)$$

In this work, the Debye temperature and Debye frequency of deformed metals were computed using equation (27) and (23).

III. RESULTS AND DISCUSSION

In figure 1 Debye temperature is plotted versus electron density parameter. Figure 1 revealed that there is agreement between computed and experimental value. The computed value of Debye temperature is lower than experimental values due to the frequency approximation by treating the atoms in a crystal as single frequency quantum harmonic oscillator and this frequency depends on the strength of the restoring force acting on the atom. The experimental values of the Debye temperature in figure 1 is more concentrated in the high density limit and is higher than the computed value of the Debye temperature. This is because there are some properties that the Debye temperature depends upon that the model does not consider such as atomic vibration, thermal excitation and the ionization energy. Figure 1 also revealed that Debye temperature of metals in the high density region is higher than the Debye temperature in the low density region. This suggest that the higher the number of valence electron in metals the higher the Debye temperature and the lower the number of valence electron in metals the lower the Debye temperature. In figure 2 Debye frequency is plotted against electron density parameter. The experimental values of the Debye frequency were obtained from Solid State Physics by Efthimios, (2003). The result obtained in figure 2 revealed that the experimental Debye frequency is greater than computed value due to short coming from mean atomic velocity, amplitude of atomic vibrations and the inter-atomic bonding of the metals. Figure 2 revealed that Debye frequency of the metals is more concentrated in the high density limit than low density limit. This seems to suggest that the Debye frequency of metals depend on number of carrier electron per unit volume. Furthermore, in figure 2 there is agreement between the computed and experimental values of the Debye frequency. In figure 3 and 4, Debye temperature and Debye frequency is plotted against deformation. The Debye temperature and Debye frequency of metals decreases as deformation increases. This shows that the electrostatic and binding forces in metals decreases as deformation increases. Figure 3 and 4 also revealed that potassium has the lowest Debye temperature and Debye frequency while molybdenum and Tunasten has the highest during deformation. This is due to high electronic energy, nature of metallic bond and variable electron in this metal. Figure 3 and 4 shows that the Debye temperature and Debye frequency is strongly affected by deformation.

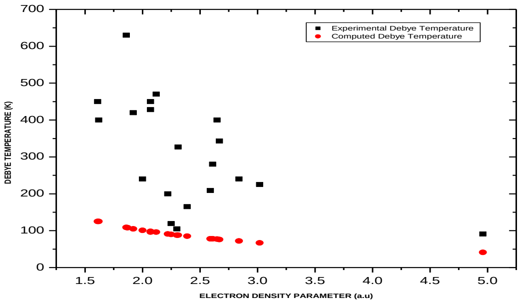


Figure 1; DEBYE TEMPERATURE VERSUS ELECTRON DENSITY PARAMETER

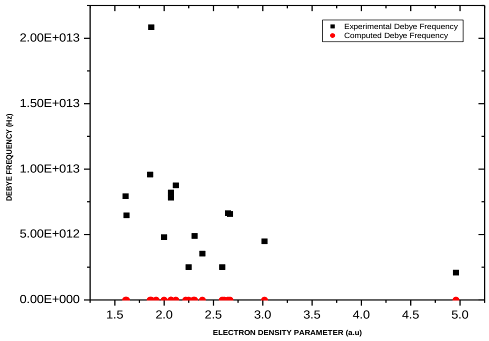
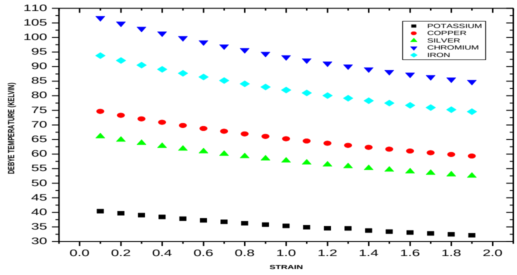
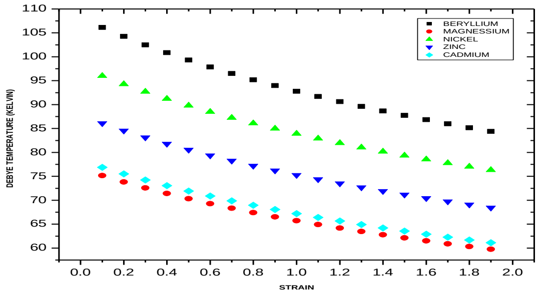
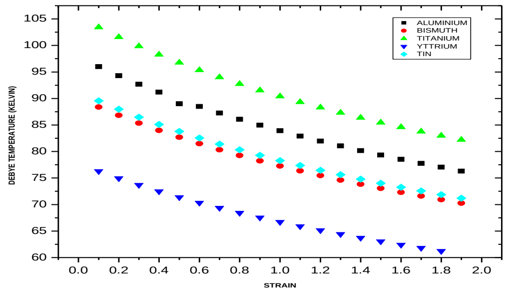


Figure 2: DEBYE FREQUENCY PLOTTED AGAINST ELECTRON DENSITY PARAMETER







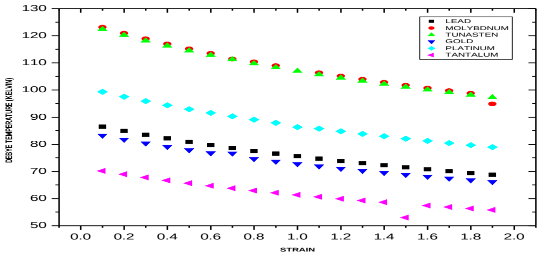
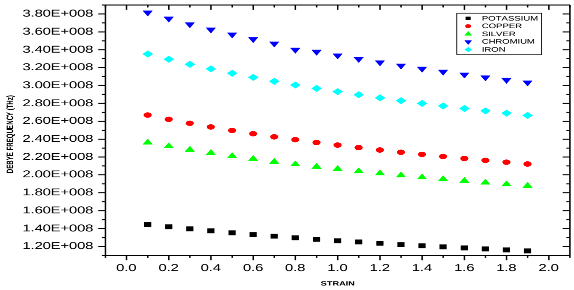
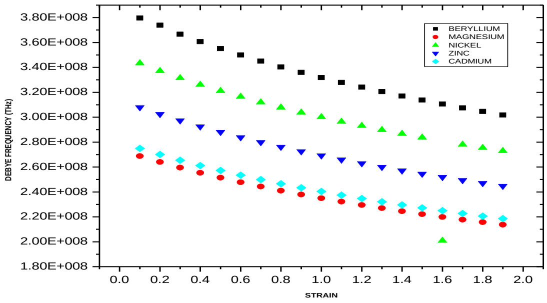
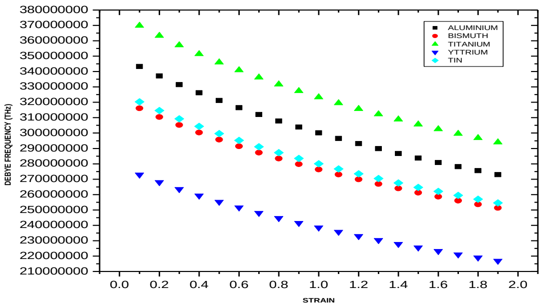


Figure 3: DEBYE TEMPERATURE PLOTTED AGAINST DEFORMATION







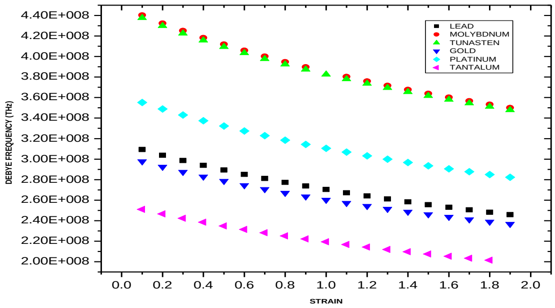
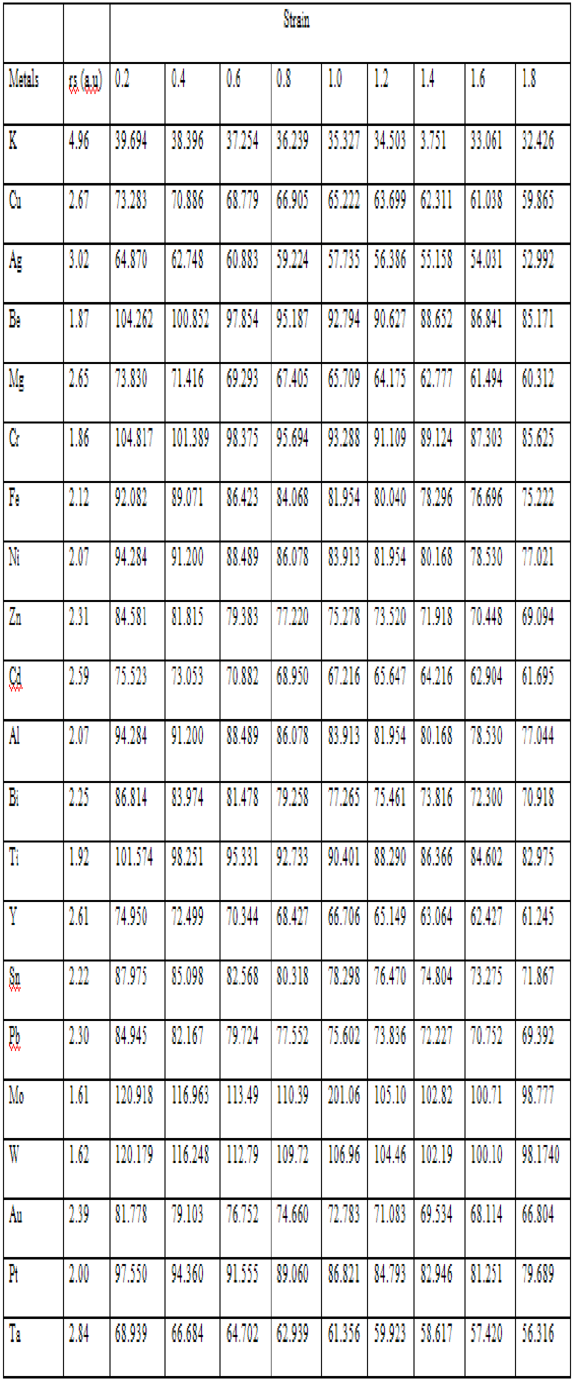


Figure 4: DEBYE FREQUENCY PLOTTED AGAINST DEFORMATION

IV. CONCLUSION

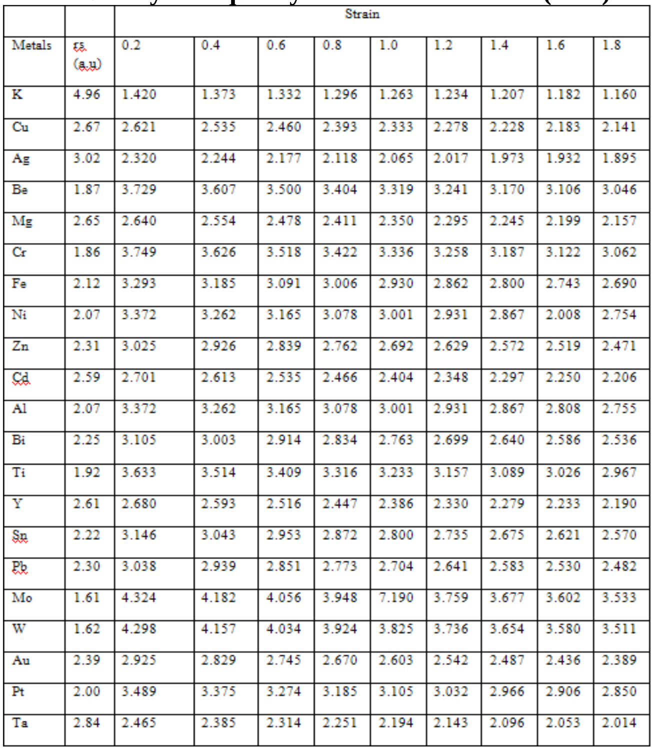
A model for computing Debye temperature and Debye frequency of metals based on the Einstein model formalism is presented. The Debye temperature and Debye frequency obtained were in agreement with experimental results which show that Einstein model is useful in the theoretical prediction of some properties of metals. Also, the computed and experimental value of Debye temperature and Debye frequency of the undeformed metals are more concentrated in the high density region. This shows that the higher the valence electron in metals the higher the Debye temperature and Debye frequency. *The Debye temperature and Debye frequency of all the metals decreases as deformation increases.*

Table 1: ***Debye Temperature of Deformed Metals (K)***



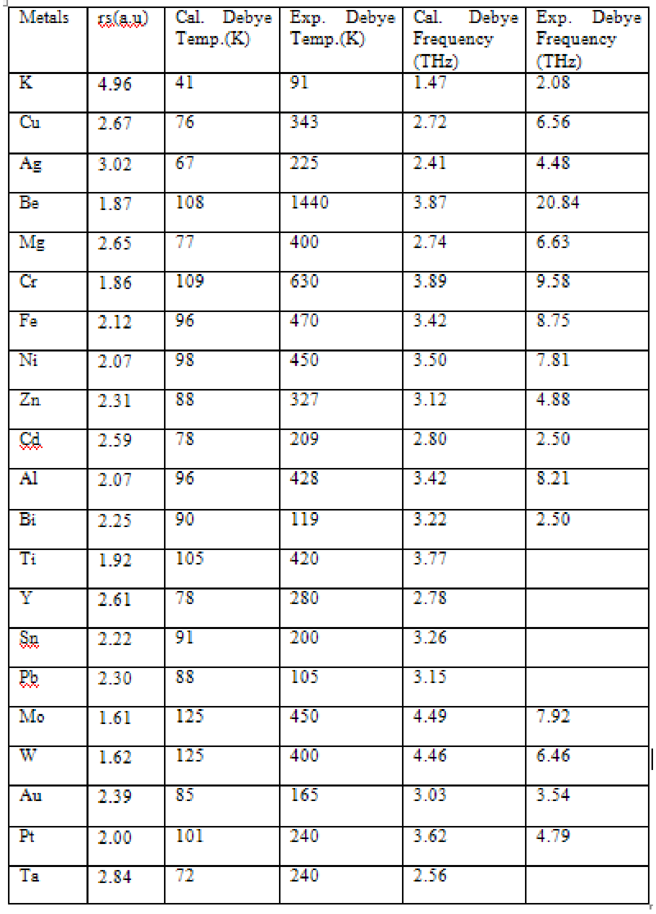
		Strain								
Metals	rs (a.u)	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8
K	4.96	39.694	38.396	37.254	36.239	35.327	34.503	3.751	33.061	32.426
Cu	2.67	73.283	70.886	68.779	66.905	65.222	63.699	62.311	61.038	59.865
Ag	3.02	64.870	62.748	60.883	59.224	57.735	56.386	55.158	54.031	52.992
Be	1.87	104.262	100.852	97.854	95.187	92.794	90.627	88.652	86.841	85.171
Mg	2.65	73.830	71.416	69.293	67.405	65.709	64.175	62.777	61.494	60.312
Cr	1.86	104.817	101.389	98.375	95.694	93.288	91.109	89.124	87.303	85.625
Fe	2.12	92.082	89.071	86.423	84.068	81.954	80.040	78.296	76.696	75.222
Ni	2.07	94.284	91.200	88.489	86.078	83.913	81.954	80.168	78.530	77.021
Zn	2.31	84.581	81.815	79.383	77.220	75.278	73.520	71.918	70.448	69.094
Cd	2.59	75.523	73.053	70.882	68.950	67.216	65.647	64.216	62.904	61.695
Al	2.07	94.284	91.200	88.489	86.078	83.913	81.954	80.168	78.530	77.044
Bi	2.25	86.814	83.974	81.478	79.258	77.265	75.461	73.816	72.300	70.918
Ti	1.92	101.574	98.251	95.331	92.733	90.401	88.290	86.366	84.602	82.975
Y	2.61	74.950	72.499	70.344	68.427	66.706	65.149	63.064	62.427	61.245
Sn	2.22	87.975	85.098	82.568	80.318	78.298	76.470	74.804	73.275	71.867
Pb	2.30	84.945	82.167	79.724	77.552	75.602	73.836	72.227	70.752	69.392
Mo	1.61	120.918	116.963	113.49	110.39	201.06	105.10	102.82	100.71	98.777
W	1.62	120.179	116.248	112.79	109.72	106.96	104.46	102.19	100.10	98.1740
Au	2.39	81.778	79.103	76.752	74.660	72.783	71.083	69.534	68.114	66.804
Pt	2.00	97.550	94.360	91.555	89.060	86.821	84.793	82.946	81.251	79.689
Ta	2.84	68.939	66.684	64.702	62.939	61.356	59.923	58.617	57.420	56.316

Table 2: Debye Frequency of Deformed Metals (THz)



		Strain								
Metals	rs (a.u)	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8
K	4.96	1.420	1.373	1.332	1.296	1.263	1.234	1.207	1.182	1.160
Cu	2.67	2.621	2.535	2.460	2.393	2.333	2.278	2.228	2.183	2.141
Ag	3.02	2.320	2.244	2.177	2.118	2.065	2.017	1.973	1.932	1.895
Be	1.87	3.729	3.607	3.500	3.404	3.319	3.241	3.170	3.106	3.046
Mg	2.65	2.640	2.554	2.478	2.411	2.350	2.295	2.245	2.199	2.157
Cr	1.86	3.749	3.626	3.518	3.422	3.336	3.258	3.187	3.122	3.062
Fe	2.12	3.293	3.185	3.091	3.006	2.930	2.862	2.800	2.743	2.690
Ni	2.07	3.372	3.262	3.165	3.078	3.001	2.931	2.867	2.008	2.754
Zn	2.31	3.025	2.926	2.839	2.762	2.692	2.629	2.572	2.519	2.471
Cd	2.59	2.701	2.613	2.535	2.466	2.404	2.348	2.297	2.250	2.206
Al	2.07	3.372	3.262	3.165	3.078	3.001	2.931	2.867	2.808	2.755
Bi	2.25	3.105	3.003	2.914	2.834	2.763	2.699	2.640	2.586	2.536
Ti	1.92	3.633	3.514	3.409	3.316	3.233	3.157	3.089	3.026	2.967
Y	2.61	2.680	2.593	2.516	2.447	2.386	2.330	2.279	2.233	2.190
Sn	2.22	3.146	3.043	2.953	2.872	2.800	2.735	2.675	2.621	2.570
Pb	2.30	3.038	2.939	2.851	2.773	2.704	2.641	2.583	2.530	2.482
Mo	1.61	4.324	4.182	4.056	3.948	7.190	3.759	3.677	3.602	3.533
W	1.62	4.298	4.157	4.034	3.924	3.825	3.736	3.654	3.580	3.511
Au	2.39	2.925	2.829	2.745	2.670	2.603	2.542	2.487	2.436	2.389
Pt	2.00	3.489	3.375	3.274	3.185	3.105	3.032	2.966	2.906	2.850
Ta	2.84	2.465	2.385	2.314	2.251	2.194	2.143	2.096	2.053	2.014

Table 3: Debye Temperature and Debye Frequency of undeformed Metals. The experimental values were obtained from Introduction to solid state Physics by Kittel (1976) and Ashcroft and Mermin (1976) .



Metals	rs(a.u)	Cal. Debye Temp.(K)	Exp. Debye Temp.(K)	Cal. Debye Frequency (THz)	Exp. Debye Frequency (THz)
K	4.96	41	91	1.47	2.08
Cu	2.67	76	343	2.72	6.56
Ag	3.02	67	225	2.41	4.48
Be	1.87	108	1440	3.87	20.84
Mg	2.65	77	400	2.74	6.63
Cr	1.86	109	630	3.89	9.58
Fe	2.12	96	470	3.42	8.75
Ni	2.07	98	450	3.50	7.81
Zn	2.31	88	327	3.12	4.88
Cd	2.59	78	209	2.80	2.50
Al	2.07	96	428	3.42	8.21
Bi	2.25	90	119	3.22	2.50
Ti	1.92	105	420	3.77	
Y	2.61	78	280	2.78	
Sn	2.22	91	200	3.26	
Pb	2.30	88	105	3.15	
Mo	1.61	125	450	4.49	7.92
W	1.62	125	400	4.46	6.46
Au	2.39	85	165	3.03	3.54
Pt	2.00	101	240	3.62	4.79
Ta	2.84	72	240	2.56	

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