

## Theoretical Study Of The Effect Of Linear Deformation On Thermal Conductivity Of Some Metal

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**Abstract:** The effects of linear deformation on thermal conductivity of different elemental metals containing monovalent, divalent, trivalent and polyvalent metals were computed and studied based on Debye model using kinetic theory of gas formalism. The electron density parameters of deformed metals under the application of different strains were obtained for different metals. The poisson ratio relating the transversal compression to elongation in the direction of applied deformation for different elemental metals were computed using elastic moduli for homogeneous isotropic material for some metal. The results obtained revealed that there is a good agreement between the computed and experimental value of the thermal conductivity of metals. There is high concentration of electron in the high density region than in the lower density region these seems to suggest that thermal conductivity of metals depend on electronic concentration. The thermal conductivity of metals increases as deformation (strains) increases for all the metals investigated. This could be due to an increase in the electron collision and inter-atomic distance between the interacting electrons in the metals which force the thermal conductivity of the metals to increase as deformation increases. The effect of deformation is more pronounced on the thermal conductivity of alkaline metals than the noble and polyvalent metal this tells us that the thermal conductivity of metals depend on electronic concentration and valence electron density.

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### 1.0 Introduction

Heat energy can be transmitted through a crystal via the motion of phonons, photons, free electron (or free holes), electron holes pairs, or excitons (bound electron hole pairs). The electronic component of heat conduction usually make the largest contribution in a metal, but almost all of the thermal current in a non metal is carried by the phonons, except at the highest temperature when the phonons becomes dominant. Heat conduction is a transport phenomenon. It is an example of a general process by which a conserved quantity (such as energy, mass, charge or momentum) is transferred as a consequence of some nonequilibrium situation in a system. Thermal conductivity is the phenomenon by which heat is transported from high to low temperature regions of a substance and is the property that characterizes the ability of a material to transfer heat (Kakani and Kakani, 2004). Thermal conductivity of metals is due to the valence electron and the magnitude of the corresponding parameters such as mean free path, Fermi velocity and electronics heat capacity (Animalu, 1977). The reciprocal of thermal conductivity is thermal resistivity. Drude assumed that the thermal conductivity of a metal originates principally from the gas of free electrons which can transfer heat with greater ease than the ions which are bound to their positions (Amit and Verbin, 1995). Thermal conductivity is actually a tensor, which means it is

possible to have different values in different directions. The electronic thermal conductivity is related to the electrical conductivity through the mean free path (Kakani and Kakani, 2004). The mean free path is the average time between consecutive collisions in the gas and is the average time during which the molecule moves as a free particle. The clarification of the concept of a mean free path and its quantitative evaluation opened the way for the calculation of many important quantities such as mobility, diffusion coefficients, viscosity and thermal conductivity. Electronic specific heat is the contribution to total specific heat due to transitions of electrons to state of higher energy. Debye temperature is one important factor in the discussion of many physical properties such as elastic constants, electrical conductivity, thermal conductivity and x-ray diffraction. The thermal properties of solid depend on energy change of the atoms and free electrons (Pillai, 2010). The specific heat at constant volume is the change in internal energy with temperature. (Elliot, 1997). Specific heat is a measure of the number of degree of freedom to absorb potential or kinetic energy (Kachhava, 1992). Deformation can be described as change in shape or size of an object due to an applied stress (force) or strain. Metals could be deformed by a compressive, elongative and torsion/twisting force. The study of the elastic behaviour of solid is very important in the

fundamental and technical researches. In technology, it tells us about the strength of the materials. In fundamental research, it is of interest because of the insight it provides into the nature of the binding forces in solids. The relevant elastic constants also relate themselves to thermal properties like Debye temperature and thermal conductivity (Kaldis, 1979). Consequently, a lot of efforts have been made to study the effect of deformation on some properties of metals theoretically and experimentally. Kiejna and Pogosov (1999) performed an experimental investigation on the effect of deformation on some electronic properties of metals by taking the direct measurement of deformed metal using Kelvin method. They observed that the contact potential difference of the metals increase when compressed and decreases when tensed. Pogosov and Shtepa, (2006), calculated the surface stress and the contact potential difference of elastically deformed metals based on structureless pseudopotential model using self-consistent Kohn Sham method. The results of surface stress obtained were in agreement with experimental results, and also confirmed that the contact potential difference obtained for the deformed metallic surfaces by Kelvin method correspond to change in surface potential. Adeshakin and Osiele (2012) computed the surface energy and surface stress of deformed metals based on the structureless pseudopotential formalism. The results obtained revealed that deformation causes a reduction of surface energy and this reduction is more pronounced in simple and alkaline metals. Tensile stress is present in most metallic surfaces whose surface stress was computed, although a few metals possess compressive stress on their surfaces. In the presence of deformation, the surface stress of some metals decreases, while deformation causes an increase in the surface stress of some metals. Adeshakin et al. (2012), developed a model based on the structureless pseudopotential formalism to compute the correlation, binding and cohesive energy of deformed and undeformed metals. The computed binding and cohesive energy of metals were compared with available experimental values. The results obtained showed that correlation energy increases with increase in electron density parameter. The computed binding energy and cohesive energy of metals were in good agreement with experimental values. The results obtained also showed that deformation causes a decrease in the binding energy of metals and it does not cause a significant change in the cohesive energy of metals, although transition metals have high values of cohesive energy compared to alkaline and simple metals. Adeshakin *et. al* (2015) investigated the linear deformation and the electronic properties of metals based on the modified structureless pseudopotential model to compute and study the effects of deformation

on the electron density parameter, Fermi energy, Fermi wave vector and chemical potential of different metals. The results obtained revealed that increase in deformation causes an increase in electron gas parameter, and decrease in Fermi wave vector, Fermi energy and chemical potential of metals. Adesakin, (2016) develop a model to compute the electrical conductivity of different elemental metals based on pseudopotential formalism. The results obtained revealed that there is a good agreement between the computed and experimental value of the electrical conductivity of metals. There is high concentration of electron in the high density region than the low density region. The electrical conductivity of metals decreases as deformation (strains) increases for all the metals investigated. The effect of deformation is more pronounced on the electrical conductivity of noble and transition metals than in alkaline metals. In this work, the thermal conductivity of undeformed and deformed elemental metals consisting of alkaline, earth alkaline, trivalent and polyvalent metals were computed based on Debye model formalism. The results obtained for the thermal conductivity of undeformed metal were compared with available experimental value to validate the model used in this work. This will provide an insight into how the thermal conductivity of metals varies with deformation. The metals were chosen based on the availability of experimental data, their industrial and technological applications, and availability of some physical constants of metals that is required for computation.

## 2.0 Theoretical Consideration

Considering a hypothetical crystal in the shape of a rectangular parallelepiped. In the undeformed state all of its faces are equivalent. Assume that deformation is a measured quantity and a metallic crystal to be considered as assembled from a number of simple crystallites. Express the average electron density in a metal as a function of deformation. Express the average electron density in a metal as a function of deformation for this purpose, consider a cubic cell of the side length  $a_o$  and volume (Kiejna and Pogosov, 1999).

$$\Omega_0 = a_o^3 = \frac{4}{3} \pi r_0^3 \quad (1)$$

where  $r_o$  is the radius of the Wigner-Seitz cell given as  $r_0 = z^{\frac{1}{3}} r_s$  where  $r_s$  is the electron density parameter of undeformed metal defined as the radius of sphere containing one electron on average and a measure of the average distance between electrons.  $r_s$  is defined as

$$r_s = \left( \frac{3}{4} \pi n \right)^{1/3} \quad (2)$$

where  $n$  is the electronic density of undeformed crystal. For a cubic cell deformed by applying an elongative force along the  $x$ -axis, the volume of the deformed cell is

$$\Omega_d = a_x a_y a_z = \frac{4}{3} \pi a b^2 \quad (3)$$

where  $a_x, a_y = a_z$  are the sides of the deformed cubic cell. If the uniaxial strain is  $u_{xx}$ , then

$$\begin{aligned} a_x &= a_0 [1 + u_{xx}] \\ a_z &= a_0 [1 + u_{zz}] = a_0 [1 - \nu u_{xx}] \end{aligned} \quad (4)$$

where  $\nu$  is the polycrystalline Poisson ratio that relates the transversal compression to the elongation in the direction of the applied deformation that is  $u_{yy} = u_{zz} = -\nu u_{xx}$

The ratio of the unit volume of the deformed cubic cell to that of the undeformed cell is

$$\frac{\Omega_d}{\Omega_0} = \frac{a_0 [1 + u_{xx}] a_0 [1 + u_{yy}] a_0 [1 + u_{zz}]}{a_0^3} \quad (5)$$

$$\frac{\Omega_d}{\Omega_0} = [1 + u_{xx}] [1 + u_{yy} + u_{zz} + u_{yy} u_{zz}] \quad (6)$$

Neglecting higher order terms of the uniaxial strain, then (Kiejna and Pogosov, 1999)

$$\frac{\Omega_d}{\Omega_0} - 1 = u_{xx} + u_{yy} + u_{zz} \quad (7)$$

From equation (4), then for the deformed cube,

$$\begin{aligned} a &= r_0 (1 + u_{xx}) \\ b &= r_0 (1 - \nu u_{xx}) \end{aligned}$$

In the same vane, the lattice spacing in the planes perpendicular to the  $y$  or  $z$  direction is

$$d_u = d_0 (1 - \nu u_{xx})$$

where  $d_0$  is the interplanar spacing in an undeformed metal given as

$$d_0 = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad (8)$$

where  $h, k$  and  $l$  are the Miller indices of the plane.

The average electron density in the deformed metal is

$$n_{av} = \frac{n_0 \Omega_0}{\Omega} = \frac{n_0 a_0^3}{a_0 (1 + u_{xx}) (a_0 (1 - \nu u_{xx}))^2}$$

$$n_{av} = n_0 [1 - (1 - 2\nu)u_{xx}] + 0(u_{xx}^2) \quad (9)$$

The electron gas parameter of the deformed metal is obtained from its volume as

$$\begin{aligned} \frac{4}{3} \pi r_{su}^3 &= \frac{4}{3} \pi a b^2 \\ r_{su}^3 &= r_0^3 (1 + u_{xx}) (r_0^2 (1 - \nu u_{xx})^2) \\ r_{su}^3 &= r_0^3 (1 + u_{xx} - \nu u_{xx} + \nu u_{xx}^2 - \nu u_{xx} - \nu u_{xx}^2) \end{aligned}$$

Neglecting higher order terms in the strain or deformation, we have (Kiejna and Pogosov, 1999)

$$r_{su} = r_0 (1 + u_{xx} (1 - 2\nu))^{1/3} \quad (10)$$

The electron gas parameter of deformed metals,  $r_{su}$  gives the mean inter electronic distance in a deformed metal (Kiejna and Pogosov, 1999).

The number of states in the blackbody radiation with frequency between  $\nu$  and  $\nu + d\nu$  is

$$g(\nu) d\nu = \frac{8\pi V}{c^3} \nu^2 d\nu \quad (11)$$

Where  $g(\nu) d\nu$  gives the number of oscillatory modes in the frequency range  $d\nu$  corresponding to the energy range  $dE$ ,  $V$  is the volume and  $c$  is the speed of light.

For the elastic transverse waves and the longitudinal waves we have

$$g_t(\nu) d\nu = \frac{8\pi V}{v_t^3} \nu^2 d\nu \quad (12)$$

And

$$g_l(\nu) d\nu = \frac{4\pi V}{v_l^3} \nu^2 d\nu \quad (13)$$

Where  $v_t$  is the velocity of the transverse wave and  $v_l$  is the velocity of the longitudinal wave. The total number of vibrational modes in the frequency range  $d\nu$  is

$$g(\nu) d\nu = g_t(\nu) d\nu + g_l(\nu) d\nu \quad (14)$$

Substituting equation (12) and (13) into equation (14) we have

$$g(\nu) d\nu = 4\pi V \left( \frac{1}{v_t^3} + \frac{2}{v_l^3} \right) \nu^2 d\nu \quad (15)$$

In a continuous medium, there is no limit to the total number of vibrational modes. But in solids that has an atomic structure and contain  $N$  atoms, any vibrational mode must be described in terms of  $3N$  positional coordinates of the atoms. This therefore imposes a limit on the total number of independent modes of freedom which must be equal to  $3N$ . where  $N$  is the number of atoms in a monoatomic homogeneous solid. This imposes a limit on the maximum vibrational frequency. Using equation (15)

$$3N = \int_0^{\nu_0} g(\nu) d\nu \quad (16)$$

Putting equation (15) into equation (16) we have

$$3N = 4\pi V \left( \frac{1}{v_t^3} + \frac{2}{v_l^3} \right) \int_0^{\nu_0} \nu^2 d\nu \quad (17)$$

$$3N = 4\pi V \left( \frac{1}{v_l^3} + \frac{2}{v_t^3} \right) \frac{v_0^3}{3} \quad (18)$$

Therefore,

$$\frac{9N}{v_0^3} = 4\pi V \left( \frac{1}{v_l^3} + \frac{2}{v_t^3} \right) \quad (19)$$

By substituting equation (19) into equation (15) we have

$$g(v)dv = \frac{9N}{v_0^3} v^2 dv \quad (20)$$

Photons are associated with the vibrational modes of solids, in thermal equilibrium photons obey Bose-Einstein statistics.

$$dn = \frac{9N}{v_0^3} \frac{v^2}{\exp \frac{hv}{KT} - 1} dv \quad (21)$$

Equation (21) is the number of photons of energy  $E = hv$  in the frequency range between  $v$  and  $v+dv$  and in thermal equilibrium with the solid lattice at temperature  $T$ . The total vibrational energy of the solid in the frequency range  $dv$  is

$$dU = Edn = hvdn = \frac{9Nh}{v_0^3} \frac{v^3}{e^{\frac{hv}{KT}} - 1} dv \quad (22)$$

The total vibrational energy of solid is obtained by integrating equation (23), then we have

$$U = \int_0^{v_0} \frac{9Nh}{v_0^3} \frac{v^3}{e^{\frac{hv}{KT}} - 1} dv \quad (23)$$

The heat capacity at constant volume is given by

$$C_v = \frac{1}{n} \frac{\partial U}{\partial t} = \frac{9N_A h^2}{v_0^3} \int_0^{v_0} \frac{v^4 \exp \frac{hv}{KT}}{(e^{\frac{hv}{KT}} - 1)^2} dv \quad (24)$$

Where,  $n$  is the number of mole,  $N_A$  is the Avogadro number,  $\hbar$  is the normalized Planck's constant,  $K$  is the Boltzmann constant,  $T$  is the temperature and  $h$  is the Planck's constant. The Debye frequency  $w_D$  and Debye temperature  $\theta_D$  is obtained as

$$w_D = \gamma (6\pi^2 \frac{N}{V})^{\frac{1}{3}} = \gamma (6\pi^2 \eta)^{\frac{1}{3}} \quad (25)$$

And

$$\theta_D = \frac{\hbar \gamma}{K_B} (6\pi^2 \frac{N}{V})^{\frac{1}{3}} = \frac{\hbar \gamma}{K_B} (6\pi^2 \eta)^{\frac{1}{3}} \quad (26)$$

Where,  $\gamma$  is the average sound velocity and the ratio  $\frac{N}{V} = \eta$  is the electronic concentration. In insulator, heat is carried entirely by phonons, but in metals heat may be transported by both electrons and phonons. The thermal conductivity  $K$  is equal to the sum of the two contributions

$$K = K_e + K_p \quad (27)$$

Where,  $K_e$  is the electronic contribution to the thermal conductivity when the Wiedemann-Franz law is satisfied, and is obtained as

$$K_e = \left( \frac{ne^2 \tau}{m} \right) T \frac{\pi^2}{3} \left( \frac{k_B}{e} \right)^2 = 2.45 \times 10^8 \left( \frac{ne^2 \tau}{m} \right) T \quad (28)$$

Where,  $\tau$  is the relaxation time,  $T$  is the temperature,  $e$  is the electronic charge,  $m$  is the electron mass and  $K_p$  is the phonons thermal conductivity which is usually neglected due to the fact that the contribution of the electrons greatly exceeds

that of the phonons because of the great concentration of electrons.

The mean free path of a conduction electron for particle between collisions is obtained as

$$l = \frac{2\pi^2 \hbar^2}{m} \left( \frac{3}{16\pi z} \right)^{\frac{2}{3}} \frac{1}{r_s^2} \quad (29)$$

Where,  $\hbar$  is the normalized Planck's constant,  $m$  is the mass of electron,  $z$  is the valency and  $r_s$  is the electron density parameter.

From the kinetic theory of gases, the expression for the thermal conductivity is obtained as

$$K = \frac{1}{3} C_v v l \quad (30)$$

Where,  $C_v$  is the heat capacity per unit volume given by equation (24),  $v$  is the average particle velocity and  $l$  is the mean free path of a particle between collisions given by equation (29). In this work, the thermal conductivity of undeformed metals were computed based on Debye model using kinetic theory of gas for monovalent, divalent, trivalent and polyvalent metals using equation (30) and how deformation affects thermal conductivity of metals is studied.

### 3.0 Results and Discussion

Figure 1 shows the variation of thermal conductivity with electron gas parameter for some elemental metals containing monovalent, divalent, trivalent and polyvalent metals. The experimental values of the thermal conductivity of metals were obtained from Solid State Physics by Charles Kittel (1976). Figure 1 revealed that the computed value of thermal conductivity of metals is higher than the experimental values of some metals while we also have some metals whose computed thermal conductivity is higher than their experimental value. This variation could be due to the number of impurity atom, deviation from equilibrium state, electronic concentration and the efficiency of the electron motion in the metals. There is a good agreement between the computed and experimental value of the thermal conductivity of the metals. This agreement is more pronounced in the high density region than the low density region. Although, both computed and experimental value of the metals whose thermal conductivity were computed and studied Figure 1 seems not to exhibit a particular trend. Figure 1 revealed that there is high concentration of electron in the high density region than low density region. This suggests that the higher the valence electron density in metals the higher the thermal conductivity of the metal and the lower the density of valence electron in metal the lower the thermal conductivity of the metal. The trend exhibited by metals in Figure 1 also revealed that in the high density region we have the alkaline and earth alkaline metals while in the low density region

we have the noble, polyvalent and the transition metals since alkaline metals has more free mobile electron in them. The trend exhibited by metals in Figure 1 also revealed that the thermal conductivity of metal depend on the electronic concentration as most of the metals whose thermal conductivity were computed and studied have most of their electron concentrated in the high density region than the low density region.

Figure 2 shows the variation of thermal conductivity with strain for some elemental metals containing alkaline, earth alkaline, group three, transition and noble metals. Figure 2 revealed that the thermal conductivity of all the metal increases as deformation increases. This seems to suggest that as deformation increases there is an increase in the electron collision and inter-atomic distance between the electrons in the metals which force the thermal conductivity of the metals to increase as deformation increases. The trend exhibited by metals in Figure 2 could also be due to the fact that as deformation increases the free electron concentration in metals also increases and there-by causes an increase in the efficiency of the electron motion of metals which forces the thermal conductivity of the metal to increase as deformation increases. The trend exhibited by metal in Figure 2 revealed that Potassium has the highest thermal conductivity while Molybdenum has the lowest thermal conductivity among all the metals subjected to different deformation. This could be due to alkaline nature of Potassium while that of Molybdenum could be due to its polycrystalline in

nature. Furthermore, the trend exhibited by Potassium and Molybdenum in Figure 2 also revealed that the thermal conductivity of metal depend on the electronic concentration, that is the higher the electronic concentration in metal the higher the effect of deformation on the thermal conductivity of the metal and the lower the electronic concentration in metal the lower the effect of deformation on the thermal conductivity of the metal. We conclude that the thermal conductivity of metals is greatly affected by deformation as metals in the high density region have low thermal conductivity while metals in the low density region have high thermal conductivity.

#### 4.0 Conclusion

The thermal conductivity of deformed metals were computed based on Debye model formalism using kinetic theory of gas. The results obtained for thermal conductivity of undeformed metals were in good agreement with the experimental values which shows the validity of the model used in the computation. The thermal conductivity of alkaline metal is the highest among all the metals subjected to different deformation. This seems to suggest that thermal conductivity of metal depend on electronic concentration. The work also revealed that the thermal conductivity of metals increases as deformation increases. The effect of deformation on thermal conductivity of metal depends not only on the density of valence electron but on free electron concentration, efficiency of electron motion and nature of the metal.

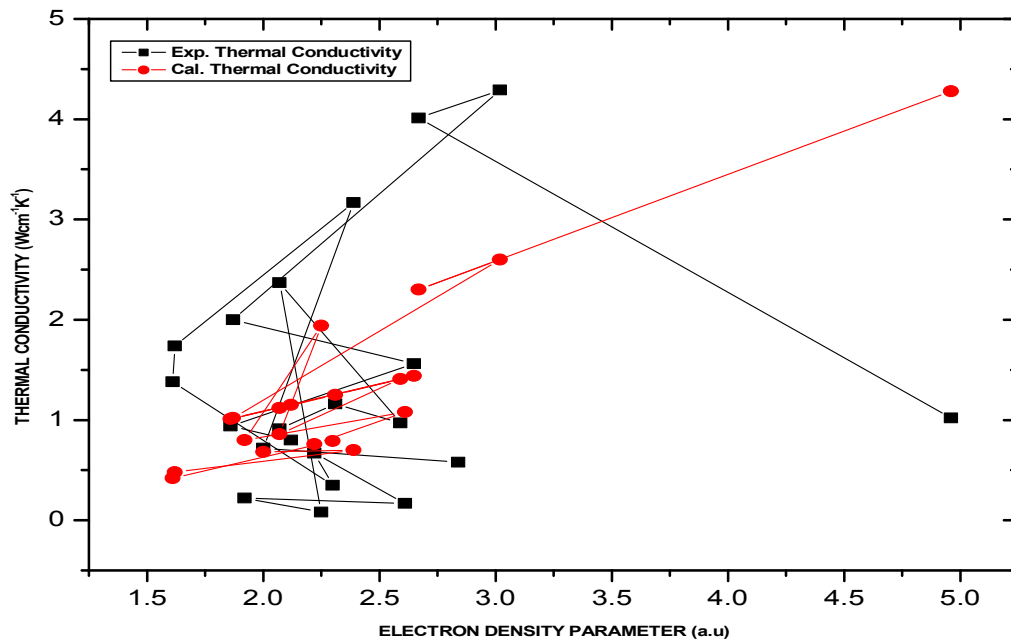
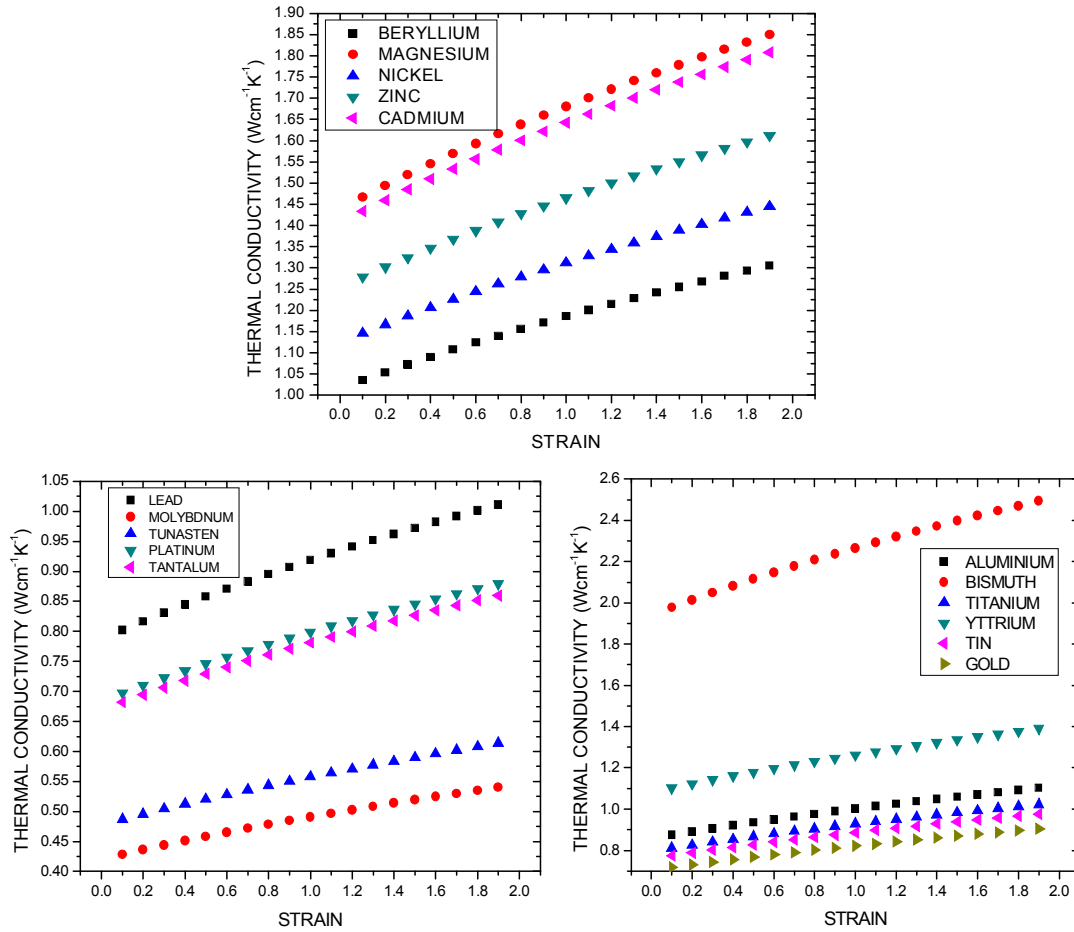


Figure 1: Variation Of Thermal Conductivity With Electron Density Parameters



**Figure 2: Variation Of Thermal Conductivity With Strain**

**Table 1: Thermal Conductivity of Deformed Metals (Wcm<sup>-1</sup>K<sup>-1</sup>)**

Metals	rs (a.u)	Strain								
		0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8
K	4.96	4.439	4.591	4.733	4.867	4.994	5.115	5.230	5.340	5.446
Cu	2.67	2.390	2.471	2.548	2.620	2.688	2.753	2.815	2.874	2.931
Ag	3.02	2.703	2.795	2.882	2.963	3.041	3.114	3.184	3.251	3.316
Be	1.87	1.054	1.090	1.124	1.156	1.186	1.214	1.242	1.268	1.293
Mg	2.65	1.494	1.545	1.593	1.638	1.680	1.721	1.760	1.797	1.832
Cr	1.86	1.049	1.084	1.118	1.150	1.179	1.208	1.235	1.261	1.286
Fe	2.12	1.195	1.236	1.274	1.310	1.344	1.377	1.408	1.437	1.466
Ni	2.07	1.167	1.207	1.244	1.279	1.313	1.344	1.375	1.404	1.431
Zn	2.31	1.302	1.347	1.388	1.428	1.465	1.500	1.534	1.566	1.597
Cd	2.59	1.460	1.510	1.557	1.601	1.642	1.682	1.720	1.756	1.791
Al	2.07	0.890	0.921	0.949	0.976	1.002	1.026	1.049	1.071	1.092
Bi	2.25	2.014	2.083	2.147	2.208	2.265	2.320	2.372	2.422	2.470
Ti	1.92	0.826	0.854	0.881	0.905	0.929	0.951	0.973	0.993	1.013
Y	2.61	1.123	1.161	1.197	1.231	1.263	1.293	1.322	1.350	1.377
Sn	2.22	0.788	0.815	0.840	0.864	0.887	0.908	0.928	0.948	0.967
Pb	2.30	0.817	0.844	0.871	0.895	0.919	0.941	0.962	0.982	1.002
Mo	1.61	0.436	0.451	0.465	0.478	0.491	0.502	0.514	0.525	0.535
W	1.62	0.496	0.513	0.528	0.543	0.558	0.571	0.584	0.596	0.608
Au	2.39	0.731	0.756	0.780	0.802	0.823	0.842	0.861	0.879	0.897
Pt	2.00	0.710	0.734	0.757	0.778	0.799	0.818	0.836	0.854	0.871
Ta	2.84	0.694	0.718	0.740	0.761	0.781	0.800	0.818	0.835	0.852

**Table 2: Thermal Conductivity ( $Wcm^{-1}K^{-1}$ ) of undeformed Metals. The experimental values were obtained from Introduction to solid state Physics by Kittel (1976).**

Metals	Electron Density Parameter $r_s$ (a.u)	Experimental Thermal conductivity at 300K	Calculated Thermal conductivity at 300K
K	4.96	1.02	4.28
Cu	2.67	4.01	2.30
Ag	3.02	4.29	2.60
Be	1.87	2.00	1.02
Mg	2.65	1.56	1.44
Cr	1.86	0.94	1.01
Fe	2.12	0.80	1.15
Ni	2.07	0.91	1.12
Zn	2.31	1.16	1.25
Cd	2.59	0.97	1.41
Al	2.07	2.37	0.86
Bi	2.25	0.08	1.94
Ti	1.92	0.22	0.80
Y	2.61	0.17	1.08
Sn	2.22	0.67	0.76
Pb	2.30	0.35	0.79
Mo	1.61	1.38	0.42
W	1.62	1.74	0.48
Au	2.39	3.17	0.70
Pt	2.00	0.72	0.68
Ta	2.84	0.58	0.67

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6/25/2017