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Effect of Linear Deformation on Electrical Conductivity of Metal

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Abstract

The effects of deformation on the electrical conductivity of different elemental metals were computed and studied based on pseudopotential formalism. The electron density parameters of deformed metals under the application of different strains were obtained for different metals. The poison ratio relating the transversal compression to elongation in the direction of applied deformation for different elemental metals were computed and used in this work. 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 in the lower density region these suggest that the higher the valence electron density in metals the higher the electrical conductivity of metals. 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 this could be due to the fact that every single valence electron in alkaline metals is free to move about with little collision between the interacting electrons which cause a strong repelling reaction in other electrons during deformation. The effect of deformation on electrical conductivity of metals also depends on the mobility, electronic concentration and nature of the metals.

Keywords: deformation, Fermi surface, resistivity, Brillouin zone, collision, pseudopotential model

1.0 Introduction

Mechanical properties of metals may be defined as the characteristics that determine the behaviour of a metal or any other material subject to applied external mechanical forces. The mechanical properties of metals include: strength, which is the resistance of the metal to deformation (Lakhtin, 1977). 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.

Electrical conductivity is the ability of a solid to conduct electric current. Electrical conductivity is proportional to number of free electrons and electron mobility (Ashcroft and Mermin, 1976). Electrical conductivity is the measure of how easily electricity flows through solids while electrical resistivity is a measure of how solids resist the flow of electricity. Electrical conductivity is inversely proportional to electrical resistivity (Borg, 1990). When conductivity is low resistivity is high and when resistivity is low, conductivity is high. Conduction in solids follows Ohms law, which states that the current is directly proportional to the electric field applied to the solids (Backofen, 1972). The concentration of free electrons plays an important role in the description of the electrical conductivity of metals (Kachhava, 1992). The electrical transport characteristic of solids is represented by the electrical conductivity defined as the constant of proportionality between the electrical current density and the electric field (Elliott, 1997). Electrical conductivity of metals is due to the movement of electrically charged particles in which the atoms in the metal elements are characterized by the presence of valence electrons in the outer shell of an atom that are free to move about. It is these free electrons that allow metals to conduct an electric current. The motion of charged elementary particles in solids is responsible for the manifestation of electrical conductivity (Pillai, 2010).The electrical conductivity of most metals is dominated at room temperature by collisions of the conduction electrons with lattice phonons. This collision rate is independent so that if the electric field were switched off the momentum distribution would relax to its ground state with the relaxation time (Kittel, 1976). For the study of electrical conductivity of solids, we do not actually need a complete knowledge of the energy bands over the entire Brillouin zone. But only electrons that may be thermally excited are affected and these lie in an energy range of the order of k_BT in width about the Fermi level (Busch and Shcade, 1976). The electrical conductivity of metals can be explained by the presence of mobile electrons in the metals. The assumption was that the free electrons in a metal could be treated as an ideal gas of free particles which in thermal equilibrium obey Maxwell-Boltzmann statistics and in the non-equilibrium state resulting from application of electric field or thermal gradients is subject to instantaneous collisions (Animalu, 1977). In solid the electrical conductivity is field independent for moderate field strengths. Different solids have very widely differing conductivities. And there is a linear relation between electrical and thermal conductivity $\frac{k}{\sigma T} = constant$ (Wiedemann-Franz law) in many metals. And there is a gross difference in the temperature dependence of electrical conductivity in metals and semiconductors (Madelung, 1978).The number of valence electrons involved in electrical conduction in a metal is practically independent of temperature. It is very interesting to note that although all the electrons participate in the conduction mechanism, the relaxation time of only those electrons which are at the Fermi level occurs in the conductivity. The conductivity is proportional to the Fermi surface area. Metals with large Fermi surface areas have high electrical conductivity. Whereas insulators with zero Fermi surface have zero conductivity. The real picture of electrical conduction in metals is quite different from the classical one, in which it was assumed that the current is carried equally by all electrons each moving with an average drift velocity. Quantum mechanical treatment shows that the current is carried out by very few electrons moving at high velocity (Pillai, 2010). The electrical conductivity of metals depends on the number of carriers per unit volume and their mobility. The way these quantities vary with temperature provides key understanding of the electrical properties of materials (Kachhava, 1992). The first classical theory of conductivity is that of Drude. All electrons are assumed to behave in the same way in an electric field. The interaction with the lattice is by collision processes in which energy and momentum are exchanged. An electron is accelerated by the external field between two collision processes. The treatment of the electrical conductivity in terms of the Drude model of a free electron gas is deficient in many respects for real metals. The Fermi-Dirac statistics governing the electron distribution are not incorporated, no physical mechanism for the electron relaxation time is considered and the Fermi surface associated with the particular crystal structure are not included (Elliott, 1997). Application of the Fermi-Dirac distribution is the clarification of the electrical conductivity and other physical properties of metals. The discovery of the Pauli principle and Fermi-Dirac distribution gives sommerfeld the tools for explaining the electrical conductivity of metals (Amit and Verbin, 1999) 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 (2000) 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. 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 were 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 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.In this work, the electrical conductivity of deformed elemental metals consisting of monovalent, divalent, trivalent and polyvalent metals were computed based on pseudopotential formalism, and the result obtained were compared with available experimental values and results obtained using other method of calculation. This will provide an insight into how the electrical conductivity of metals varies with deformation. The metals used in this study 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)

$$\Omega_0 = a_0^3 = \frac{4}{3}\pi r_0^3 \tag{1}$$

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

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

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

$$\Omega_d = a_x a_y^2 = \frac{4}{3}\pi a b^2 \tag{3}$$

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

$$\begin{aligned} a_x &= a_0\left[1+u_{xx}\right] \\ a_z &= a_0\left[1+u_{zz}\right] = a_0\left[1-\upsilon u_{xx}\right] \end{aligned} \tag{4}$$

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

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

$$\frac{\Omega_d}{\Omega_0} = \frac{a_0\left[1+u_{xx}\right]a_0\left[1+u_{yy}\right]a_0\left[1+u_{zz}\right]}{a_0^3} \tag{5}$$

$$\frac{\Omega_d}{\Omega_0} = \left[1+u_{xx}\right]\left[1+u_{yy}+u_{zz}+u_{yy}u_{zz}\right] \tag{6}$$

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

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

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

$$a = r_0(1+u_{xx})$$

$$b = r_0(1-\upsilon u_{xx})$$

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

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

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

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

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

The average electron density in the deformed metal is

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

$$n_{av} = n_0\left[1-(1-2\upsilon)u_{xx}\right] + 0(u_{xx}^2) \tag{9}$$

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

$$\frac{4}{3}\pi r_{su}^3 = \frac{4}{3}\pi a b^2$$

$$r_{su}^3 = r_0(1+u_{xx})(r_0^2(1-\upsilon u_{xx})^2)$$

$$r_{su}^3 = r_0^3\left(1+u_{xx}-\upsilon u_{xx}+\upsilon u_{xx}^2-\upsilon u_{xx}-\upsilon u_{xx}^2\right)$$

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

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

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

The spacing between the lattice planes perpendicular to the elongation and z direction is

$$d_u = d_0\left(1-\upsilon u_{xx}\right) \tag{11}$$

where d_0 is the interplanar distance, υ is the poisson ratio that is relates the transversal compression to elongation in the direction of applied deformation, u_{xx} is the uniaxial strain.

For N electrons in a volume V, all moving with the same velocity $\vec{V}$, the current density j by definition is

$$j = -\left(\frac{N}{V}\right)e\vec{V} = -ne\vec{V} \tag{12}$$

where n is the electronic concentration and e is electronic charge. Assuming that a distribution of drift velocities, the current density j_z in the z-direction is obtained by summing the electron contribution over all carriers in reciprocal space is

$$j_z = -\int eV_z \mathrm{dn} = -\frac{e}{4\pi^3}\int V_z f(\vec{k})d^3k = -\frac{e}{4\pi^3}\int V_z f_1 d^3k \tag{13}$$

The equilibrium distribution does not contribute to the current density in equation (13)

where $f_1 = e\tau EV_z\frac{\partial f_0}{\partial\varepsilon}$ (14)

substituting for f_1 in equation (13) and setting $V_z = V\cos\theta$ and integrating over θ and φ we have

$$j_z = -\frac{e^2E}{4\pi^3}\int V_z^2\tau\left(\frac{\partial f_0}{\partial\varepsilon}\right)d^3k \tag{15}$$

$$j_z = -\frac{e^2E}{4\pi^3}\int_0^\infty\int_0^\pi\int_0^{2\pi}(V\cos\theta)^2\tau\left(\frac{\partial f_0}{\partial\varepsilon}\right)k^2\sin\theta d\theta d\varphi dk \tag{16}$$

$$j_z = -\frac{e^2E}{3\pi^2}\int_0^\infty V^2\tau\left(\frac{\partial f_0}{\partial\varepsilon}\right)k^2\,dk \tag{17}$$

$$j_z = -\frac{2e^2E}{3\pi^2 m_e}\int_0^\infty \varepsilon\tau\left(\frac{\partial f_0}{\partial\varepsilon}\right)k^2\,dk \tag{18}$$

where $V^2 = {}^{2\varepsilon}/_{m_e}$ and $\varepsilon = {}^{\hbar^2k^2}/_{2m_e}$

using the parabolic energy dependence equation (18) can be written as

$$j_z = -\frac{2(2m_e)^{1/2}e^2\tau_F E}{3\pi^2\hbar^3}\int_0^\infty \varepsilon^{\frac{3}{2}}\frac{\partial f_0(\varepsilon)}{\partial\varepsilon}\,d\varepsilon \tag{19}$$

Using a function which vanishes when ε vanishes, it is common practice to introduce the integral

$$I = \int_0^\infty f(\varepsilon)\frac{\partial F(\varepsilon)}{\partial\varepsilon} = [f(\varepsilon)F(\varepsilon)]_0^\infty - \int_0^\infty F(\varepsilon)\frac{\partial f(\varepsilon)}{\partial\varepsilon} = -\int_0^\infty F(\varepsilon)\frac{\partial f(\varepsilon)}{\partial\varepsilon}d\varepsilon \tag{20}$$

$$j_z = \frac{(2m_e)^{\frac{1}{2}}e^2\tau_F E}{\pi^2\hbar^2}\int_0^\infty \varepsilon^{\frac{1}{2}} f_0(\varepsilon)d\varepsilon \tag{21}$$

where $\frac{\partial f_0}{\partial\varepsilon}$ has an appreciable value only if ε is close to the Fermi energy. τ_F can be interpreted as the effective value of the relaxation time at the Fermi level.

The electron density of state is obtained as

$$N(\varepsilon) = \frac{2V}{(2\pi)^3}\frac{4\pi k^2}{|\nabla_k\varepsilon|} = \frac{V}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)k = \frac{V}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}\varepsilon^{1/2} \tag{22}$$

The integral over all the occupied states is equal to

$$N = \int_0^\infty f(\varepsilon)\,N(\varepsilon)d\varepsilon \tag{23}$$

Using equation (22) and (23) equation (21) becomes

$$j_z = \frac{(2m_e)^{\frac{1}{2}}e^2\tau_F E}{\pi^2\hbar^2}\frac{2\pi^2}{V}\left(\frac{\hbar^2}{2m_e}\right)^{\frac{3}{2}}\int_0^\infty N(\varepsilon)\,f_0(\varepsilon)dE$$

$$j_z = \frac{N}{V}\frac{e^2\tau_F}{m_e}\,E \tag{24}$$

The proportionality constant between the current density and the applied field is

$$\sigma = \frac{N}{V}\frac{e^2\tau_F}{m_e} = \frac{ne^2\tau_F}{m_e} \tag{25}$$

The relaxation time τ_F is obtained as

$$\tau_F = \frac{\Lambda}{V_F} \tag{26}$$

where Λ is the deformed mean free path of a conduction electron obtained as

$$\Lambda = \frac{2\pi^2\hbar^2}{me}\left(\frac{3}{16\pi z}\right)^{2/3}\frac{1}{r_{su}^2} \tag{27}$$

and V_F is the Fermi Velocity of the conduction electron obtained as

$$V_F = \frac{\hbar}{me}\left(\frac{9\pi}{4}\right)^{\frac{1}{3}}\frac{1}{r_{su}} \tag{28}$$

Putting equation (27) and (28) into equation (26) we obtain

$$\tau_F = \frac{\pi\hbar}{2}\left(\frac{1}{z}\right)^{2/3}\frac{1}{r_{su}} \tag{29}$$

Substituting equation (29) into (25) we obtain the electrical conductivity of deformed metals as

$$\sigma = \frac{N}{V}\frac{e^2\tau_F}{m_e} = \frac{\pi\hbar n e^2}{2m_e}\left(\frac{1}{z}\right)^{2/3}\frac{1}{r_{su}} \tag{30}$$

Where n is electronic concentration, e is electronic charge, m_e is the mass of electron, τ_F is the relaxation time, r_{su} is electron density parameter of deformed metal and σ is the electrical conductivity.

In this work, the electrical conductivity of deformed metals for monovalent, divalent, trivalent and polyvalent metals were computed using equation (30) and how deformation affects these properties of metals is studied.

3.0 Results and Discussion

Figure 1 shows the variation of electrical conductivity with electron gas parameter for some elemental metals containing group one, group two, group three, transition and noble metals. The experimental values of the electrical conductivity of metals were obtained from Kittel (1976). Figure 1 revealed that the computed value of electrical conductivity of metals is higher than that of the experimental values. This could be due to the fact that there are some properties of metals which the electrical conductivity of metals depends upon that the model used in the computation does not take into consideration, such as thermal vibration, impurity atoms, crystalline defects and some Fermi surface properties of metals. There is a good agreement between the computed and experimental value of the electrical conductivity of metals as the metals does not exhibit a particular trend. The agreement between computed and experimental values is more pronounce between the metals in the low density region. The trend exhibited by metals in Figure 1 revealed that the higher the valence electron density in metals the higher the electrical conductivity of the metal and the lower the density of valence electron in metal the lower the electrical conductivity of the metal. Figure 1 also revealed that there is high concentration of mobile electron in the high density region than in the low density region. This suggest that in the high density region we have the alkaline and earth alkaline metals while in the low density region we have the noble and the transition metals since every single valence electron in alkaline metals is free to move and cause a strong repelling reaction in other electrons.

Figure 2 shows the variation of electrical conductivity with strain for some elemental metals containing alkaline, earth alkaline, group three, transition and noble metals. Figure 2 revealed that the electrical conductivity of all the metal decreases as deformation increases. This seems to suggest that as deformation increases there is an increase in the inter-atomic spacing/distance between the electrons in metals therefore increases the temperature and the imperfection/crystal defects of metals which force the electrical conductivity of all the metals to decrease as deformation increases. Table 2 revealed that potassium has the lowest electrical conductivity while chromium has the highest electrical conductivity among all the metals that is subjected to different deformation. This seems to suggest that the higher the electron concentration and charge carrier mobility in metal the lower the effect of deformation on the metal and the lower the electron concentration and charge carrier mobility in metal the higher the effect of deformation on the metal. Also, the trend exhibited by Potassium in Figure 2 could be due to the fact that metals with high electronic concentration has low Fermi surface while metals like Chromium with low electronic concentration are having high Fermi surface this causes their electrical conductivity to be high when subjected to deformation. The trend exhibited by the transition metals in Figure 2 could be due to high collision rate between the interacting electrons during deformation. The electrical conductivity of metals is greatly affected by deformation as metals in the high density region have high electrical conductivity while metals in the low density region have low electrical conductivity. We conclude that the electrical conductivity of metals is greatly affected by deformation.

4.0 CONCLUSION

The electrical conductivity of deformed metals were computed based on the pseudopotential formalism. The results obtained for electrical conductivity of undeformed metals were in agreement with the experimental values which shows the validity of the model used in the computation. The electrical conductivity of alkaline metal is least affected by deformation unlike noble and transition metal. The work revealed that the electrical conductivity of metals decreases with increase in deformation. The effect of deformation on electrical conductivity of metal depends not only on the density of valence electron but on mobility, carrier concentration and the nature of the metals.

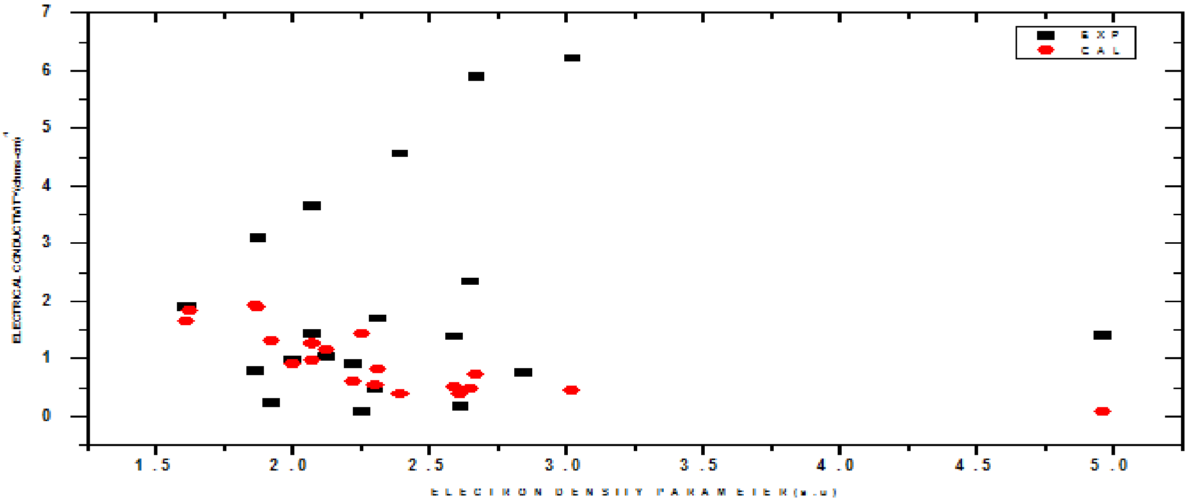

Fig. 1: Variation of Electrical Conductivity with Electron Gas Parameter for Metals

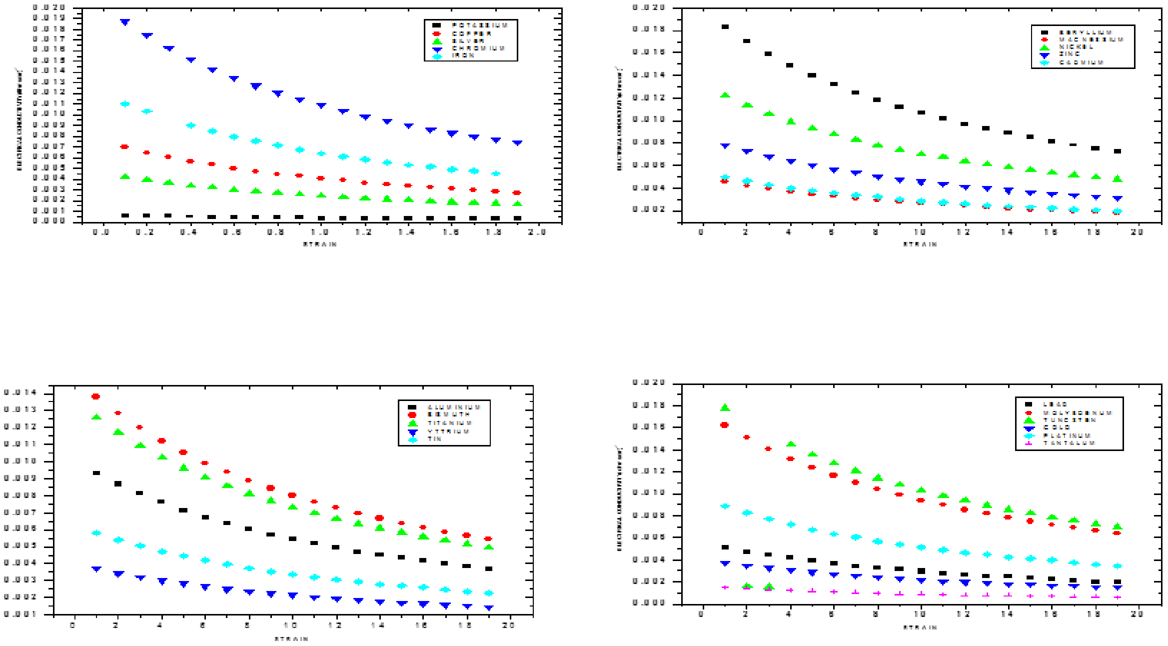

Fig. 2: Variation of Electrical Conductivity with Strain for Some Metals

Table 1: Electrical Conductivity of undeformed metals. The experimental values of Electrical Conductivity were obtained from Kittel (1976).

Metals	Electron Density Parameter r_s(a.u)	Experimental Electrical Conductivity (Ohms-cm)$^{-1}$	Calculated Electrical Conductivity (Ohms-cm)$^{-1}$
K	4.96	1.39	0.06
Cu	2.67	5.88	0.72
Ag	3.02	6.21	0.44
Be	1.87	3.08	1.89
Mg	2.65	2.33	0.47
Cr	1.86	0.78	1.93
Fe	2.12	1.02	1.14
Ni	2.07	1.43	1.26
Zn	2.31	1.69	0.81
Cd	2.59	1.38	0.51
Al	2.07	3.65	0.96
Bi	2.25	0.086	1.43
Ti	1.92	0.23	1.29
Y	2.61	0.17	0.38
Sn	2.22	0.91	0.60
Pb	2.30	0.48	0.52
Mo	1.61	1.89	1.65
W	1.62	1.89	1.82
Au	2.39	4.55	0.38
Pt	2.00	0.96	0.91
Ta	2.84	0.76	0.15

Table 2: Electrical Conductivity of Deformed Metals (ohms-cm)$^{-1}$ Equation.

		Strain								
Metals	**$r_{s\,(a.u)}$**	**0.2**	**0.4**	**0.6**	**0.8**	**1.0**	**1.2**	**1.4**	**1.6**	**1.8**
K	4.96	5.383	4.705	4.163	3.723	3.358	3.051	2.791	2.567	2.373
Cu	2.67	6.450	5.638	4.989	4.461	4.023	3.656	3.344	3.076	2.843
Ag	3.02	3.936	3.440	3.044	2.722	2.455	2.231	2.041	1.877	1.735
Be	1.87	1.703	1.488	1.317	1.177	1.062	9.65	8.83	8.12	7.50
Mg	2.65	4.207	3.677	3.254	2.909	2.624	2.385	2.181	2.006	1.855
Cr	1.86	1.740	1.520	1.345	1.203	1.085	9.86	9.02	8.30	7.67
Fe	2.12	0.010	0.009	0.008	0.007	0.006	0.006	0.005	0.005	0.005
Ni	2.07	0.011	0.010	0.009	0.008	0.007	0.006	0.006	0.005	0.005
Zn	2.31	0.007	0.006	0.006	0.005	0.005	0.004	0.004	0.003	0.003
Cd	2.59	0.005	0.004	0.004	0.003	0.003	0.003	0.002	0.002	0.002
Al	2.07	0.009	0.008	0.007	0.006	0.005	0.005	0.004	0.004	0.003
Bi	2.25	0.013	0.011	0.010	0.009	0.008	0.007	0.007	0.006	0.006
Ti	1.92	0.012	0.010	0.009	0.008	0.007	0.007	0.006	0.006	0.005
Y	2.61	0.003	0.003	0.003	0.002	0.002	0.002	0.002	0.002	0.002
Sn	2.22	0.005	0.005	0.004	0.004	0.003	0.003	0.003	0.003	0.002
Pb	2.30	0.005	0.004	0.004	0.003	0.003	0.003	0.002	0.002	0.002
Mo	1.61	0.015	0.013	0.012	0.001	0.009	0.009	0.008	0.007	0.007
W	1.62	0.002	0.014	0.013	0.011	0.010	0.009	0.009	0.008	0.007
Au	2.39	0.003	0.003	0.003	0.002	0.002	0.002	0.002	0.002	0.002
Pt	2.00	0.008	0.007	0.006	0.006	0.005	0.005	0.004	0.004	0.004
Ta	2.84	0.001	0.001	0.001	0.0010	0.0009	0.0008	0.0007	0.0007	0.0006

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