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# LINEAR DEFORMATION AND THE ELECTRONIC PROPERTIES OF METALS

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**ABSTRACT:** *In this work, the modified structureless pseudopotential model was used 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 structureless pseudopotential model was modified for deformed metals by first computing the electron density parameter of deformed metals under the application of different strains. The results obtained revealed that increase in deformation (strain) causes an increase in electron gas parameter, decrease in Fermi wave vector, Fermi energy and chemical potential of metals. The effect of deformation on electron gas parameter is more pronounced in simple metals than in transition and noble metals. The effect of deformation on Fermi wave vector depends on the elastic properties of the metals. Unlike simple metals, the Fermi energy and chemical potential of transition and noble metals are highly affected by deformation. The results of this work show the versatility of the structureless pseudopotential formalism in computing not only the properties of metals even that of deformed metals.*

**KEYWORDS**: Structureless Pseudopotential Formalism, Deformation, Metals, Electronic Properties.

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## INTRODUCTION

Deformation is described as change in shape or size of an object due to an applied stress (force). In metals, deformation can be as a result of tensile, shear, torsion or compressive force and it can be elastic or inelastic. In the range of elastic deformation, a uniaxially strained metallic sample leads to a linear change in the contact potential difference, in this range, the general statement of the theory of elasticity holds. In electronics, the area over which a stress is applied is generally very much smaller. The electronic structure is at a momentous stage with rapid advances in basic theory, new algorithms and computational methods. It is feasible to determine many properties of materials directly from the fundamental equations for the electrons and to provide new insight into vital problems in solids. Electronic structure calculations are tools used by both experimentalists and theorists to understand characteristic properties of matter and to make specific predictions for real materials and experimental observable phenomena [1].The Fermi energy is determined by the electron density or the atomic density if there is a contribution of just one valence electron per atom to the free electron gas as for alkali metals [2]. Electrons and nuclei are the fundamental particles that determine the nature of the matter of our everyday world. Not only do electrons form the “quantum glue” that holds the nuclei in solid, liquid and molecular states together, electron excitations also determine the vast array of electrical, optical and magnetic properties of materials. Strain plays a vital role in the stability of materials. Strain is a deformation that causes displacement, which in turn, affects the electronic properties of solids. The displacement, as a function of the coordinate specifies the deformation [3].

A homogeneous system is completely specified by its density, which can be characterized by the electron density parameter, $r_s$ defined as the radius of a sphere containing one electron per unit volume.The electron density parameter is a measure of the average distance between electrons.

The result of an experimental investigation on the effect of deformation on some electronic properties of metals taking direct measurement of metal deformation using Kelvin method [4], revealed that the contact potential difference of metal decreases when tensed and increases when compressed. A similar effect on the contact potential difference was observed at the surface of sample with a non-uniform distribution of residual mechanical stress[5]. Experimental work on the influence of deformation upon electronic emission from a thin metallic filmrevealed that in the range of elastic deformation, a uniaxial strain of metallic sample leads to a linear change in the contact potential difference [6, 7]. The results in this study also showed that work function increases with decreasing electron density caused by a uniaxial tension or compression of metallic sample. From the theory of elasticity, the change in total energy of a solid is proportional to the square of relative deformation and the energy must increase for compression as well as for tension.

An essential feature determining the electronic properties of any metal is the topology of the Fermi surface. In metals, there are many states whose energy is equal to Fermi energy. Since the energy of each state is a continuous function of the wave vector k, the relation $E_i(k) = E_F$ describes a continuous surface in k-space, which separates the region of occupied from the region of unoccupied states. This region of separation is called the Fermi surface. The Fermi surface is the surface of constant energy, $E_F$ in k-space which separates the filled and unfilled orbital at absolute zero temperature. The Fermi wave vector is referred to as the wave vector of the Fermi energy [8]. The Fermi energy is the energy of the highest filled state in the highest filled energy band which contains electrons in a metal at absolute zero. Fermi energy at absolute zero equals the chemical potential, which is defined as the change in energy of a thermodynamic electronic system of N particles when one extra electron is added to it.

In the present study, a modified structureless pseudopotential formlism will be used to test the effect of linear deformation on the electronic properties of metals.

## THEORETICAL CONSIDERATION

### Electron gas parameter of deformed metals

Considering a hypothetical crystal in the shape of a rectangular parallelepiped, in the normal state, all 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. For this purpose, consider a cubic cell of the side length $a_o$ and volume

$$\Omega_0 = a^3{}_0 = \frac{4}{3}\pi r_0^3 \qquad (1)$$

where $r_o$ is the radius of the Wigner-Seitz cell given as $r_0 = z^{\frac{1}{3}} r_s$ and $r_s$ 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

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

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

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

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

$$a_x = a_0[1 + u_{xx}]$$

$$a_z = a_0[1 + u_{zz}] = a_0[1 - \upsilon u_{xx}] \qquad (4)$$

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 un-deformed cell is

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

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

Neglecting higher order terms of the uniaxial strain, then

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

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

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

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

In the same vain, 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 un-deformed metal given as

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

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

The average electron density in the deformed metal is

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

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

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

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

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

Neglecting higher order terms in the strain or deformation, we have

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

The electron gas parameter of deformed metals, $r_{su}$ gives the mean inter electronic distance in a deformed metal.

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, $\upsilon$ is the Poisson ratio that is relates the transversal compression to elongation in the direction of applied deformation, $u_{xx}$ is the uniaxial strain.

## Effect of Strain on the Fermi energy of Deformed metals

The behaviour of electrons in the deformed metal is governed by the Schrodinger time independent equation

$$\frac{\hbar^2}{2m}\nabla^2\Psi + E\Psi = 0 \tag{12}$$

The normalized solution of equation (12) has the form

$$\Psi = \left(\frac{8}{\Omega}\right)^{1/2} sin\left(\frac{n_x\pi}{a_x}\right) sin\left(\frac{n_y\pi}{a_y}\right) sin\left(\frac{n_z\pi}{a_z}\right) \tag{13}$$

The eigenvalues are given by

$$\gamma = \frac{2mE}{\hbar^2} = \pi^2\left(\frac{n_x^2}{a_x^2}+\frac{n_y^2}{a_y^2}+\frac{n_z^2}{a_z^2}\right) \tag{14}$$

or by

$$\gamma = k_x^2+k_y^2+k_z^2 = |k|^2$$

where $k_x$, $k_y$, $k_z$ are the components of the wave vector k . In computing the quantities that requires summation over the wave vector, k the summation over k is replaced by integration according to the transformation

$$\sum_k \rightarrow \frac{2\Omega^3}{(2\pi)^3}\int d^3k$$

The factor of two appearing in the denominator comes from the spin, According to Pauli exclusion principle, two one-electron states with opposite spins can be assigned to every k-point. In the ground state, each of the states up to the maximum, $k_{max}$ is occupied by two electrons filling a sphere in k-space of radius $k_{max}$ called Fermi sphere. For the system of N free electrons in the volume, Ω, the average electronic density $n_{ave}$ in terms of $k_f$ is

$$n_{ave} = \frac{N}{\Omega} = \frac{k_f}{3\pi^2} \tag{15}$$

The energy of the highest occupied state at absolute zero temperature is called the Fermi energy expressed as

$$E_f = \frac{\hbar^2 k_f^2}{2m} = \frac{\hbar}{2m}(3\pi n_{ave})^{2/3} \tag{16}$$

The electron gas parameter, $r_{su}$ of the deformed metal is defined as

$$\frac{4\pi}{3} r_{su}^3 = \frac{\Omega}{N}$$

The Fermi wave vector $k_f$ and the Fermi energy $E_f$ of deformed metals in terms of the electron gas parameter, $r_{su}$ is obtained as

$$k_f = \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{r_{su}} \tag{17}$$

and

$$E_f = \frac{me^4}{2\hbar^2}\left(\frac{9\pi}{4}\right)^{2/3}\left(\frac{1}{r_{su}^2}\right) \tag{18}$$

## Chemical Potential of Deformed Metals

The energy functional of a jellium model is (Kiejna et al., 1993)

$$E_J = T_s[n] + E_{xc}[n] + \frac{1}{2}\int d^3 r\varphi([n,n_+],r[n(r)-n_+(r)] \tag{19}$$

Since, there is a deficiency in the jellium model which makes it unstable at high electronic concentration and also gives a negative surface energy due to the over estimation of kinetic energy. This is corrected by the addition of the stabilized jellium model as shown in the equation $E[n,n_{++}] = E_J[n,n_+] + (E_m + W_R)\int d^3 r n_+(r) + <\delta v>_{WS} \int d^3 r\theta(r)[n(r)-n_+(r)]$ (20)

where $T_s[n]$ and $E_{xc}[n]$ are the respective kinetic and exchange-correlation energies. $\theta([n,n_+],r)$ is the electrostatic potential of the jellium. $E_m$ is the Madelung energy; $W_R$ is the short range repulsive potential of the ionic potential and $\theta(r)$ is the unit function

The energy of the stabilized jellium can be written as

$$E = t_s + \varepsilon_{ex} + \varepsilon_{corr} + w_R + \varepsilon_M \quad (21)$$

where $t_s$ and $\varepsilon_{ex}$ are the respective kinetic and electrostatic energies in the low density approximation of the density functional theory, $\varepsilon_{corr}$ is the correlation energy. The correlation energy of deformed metals used in this work was obtained from that of undeformed metals proposed by [9] and parameterized by [10] and is expressed as

$$\varepsilon_e = \frac{-0.1423}{1+1.0529 r_{su}^{\frac{1}{2}} + 0.3334 r_{su}} \qquad (22)$$

The chemical potential, which is the change in the energy of the system as a result of the addition of an electron is obtained as

$$\mu = \frac{1}{r_{su}} \frac{dE}{dr_{su}} \qquad (23)$$

In this work, the electron gas parameter, Fermi energy, and chemical potential of deformed metals is computed and studied. The effects of strain on these electronic properties of deformed metals will be studied inorder to gain an insight into how deformation affects these electronic properties of metals.

## RESULTS AND DISCUSSION

The variation of the computed electron gas parameter with strain for different metals is shown in Figure 1. The electron gas parameter varies in the same manner for all the metals as the strain causes an increase in the electron gas parameter of all the metals investigated. The figure also revealed that of all the metals investigated,Potassium has the highest electron gas parameter. This indicates that the applied strain acts directly on the electronic concentration of the deformed metals. Molybdenum and Tungsten has the lowest electron gas parameter of the all the deformed metals investigated, this seems to suggests that the electron gas parameter of transition metals are slightly affected by deformation compared to that of simple metals. This may be due to the strong binding force between the electrons in the transition metals. The increase in electron gas parameter with strain or deformation may be due to the fact the strain causes an increase in the atomic volume which the electron gas parameter depends inversely on. The result obtained in this study for the variation of electron gas parameter of the deformed metals is in agreement with previous predictions [11, 12].

Figure 2 shows the variation of Fermi wave vector of undeformed metals with electron gas parameter for some metals. The Fermi wave vector decreases with an increase in the electron gas parameter as metals in the high density limit has high values of the Femi wave vector while metals in the low density limit has low values of the Fermi wave vector. This seems to suggest that electrons in metals in the high density limit have lower polarizability and higher Fermi wave vector while electrons in metals in the low density limit have high polarizability and low Fermi wave vector. The trend exhibited by the Fermi wave vector of metals suggests that the

Fermi wave vector of metals depends inversely on the valence electron concentration of the metals.

Figure 3 shows the variation of Fermi wave vector with deformation for some metals. As shown in the figure, the Fermi wave vector decreases with an increase in deformation for all the metals investigated with the metals in the high density region having high Fermi wave vector while metals in the low density region has low values of the Fermi wave vector. The rate of decrease of the Fermi wave vector varies depending on the nature of the metal. For some metals, (Gold, Lead, Potassium, and Copper) the rate of decrease is linear, but for some metals like Chromium, Molybdenum, Tungsten, Beryllium the rate of decrease is rather parabolic. This could be due to the elastic properties of the metals. Molybdenum and Tungsten has the highest Fermi wave vector while potassium has the lowest Fermi wave vector. Hence, Fermi wave vector depends inversely on the electronic concentration of metals. The trend exhibited by the Fermi wave vector of the deformed metals seems to suggest that deformation reduces the Fermi wave vector of metals.Furthermore, the Fermi wave vector of metals is highly affected by deformation as the packing density of metals decreases with increase in deformation.

Figure 4 shows the variation of computed and experimental Fermi energy with electron gas parameter. The experimental values of Fermi energy of metals were obtained from [13, 14].The Fermi energy of metals decreases with an increase in the electron gas parameter and there is a one to one agreement between the computed and experimental Fermi energy of metals. As shown in the Figure, for $r_s>3.0$ a.u (low density region) there is a good agreement between the computed Fermi energy of metals and experimental values. The agreement between the computed Fermi energy and experimental values for metals in this region may be due to the accuracy of the model in accounting for the Fermi energy of metals, since the model took into consideration all the properties of the metals that the Fermi energy depends on.

In Figure 5, the Fermi energy of metals decreases with an increase in deformation with the decrease being more pronounced in the transition and inner transition metals. Molybdenum and Tungsten showed the greatest variation of Fermi energy with deformation while deformation does not significantly affect the Fermi energy of Potassium. This seems to suggest that the elastic properties of metals affect their Fermi energy. Furthermore, the result showed that the higher the electronic concentration of metals, the higher the effect of deformation on its Fermi energy. The reductions of the Fermi energy as a result of deformation suggest that the applied deformation causes the Fermi energy to shift downward. The shifting downward of the Fermi energy depends on the electronic concentration of the metals.

The variation of chemical potential with electron gas parameters of some elemental metals is shown in Figure 6. Metals in the high density limit have high values of chemical potential while metals in the low density limit have low values of the chemical potential. This reveals that the change in the energy of a metal resulting from the addition of an atom to the metal depends directly on the electronic concentration of the metal. The variation of chemical potential with deformation (strain) for some metals as shown in Figure 7 reveals that increase in strain causes a reduction in the chemical potential of the metals. The chemical potential of simple metals is least affected by deformation. The effect of deformation on chemical potential of metals is more pronounced for transition and noble metals. This may be due to the type of bonding that prevails in these metals.

## CONCLUSION

The electron density parameter, Fermi energy, Fermi wavevector and chemical potential of deformed metals were computed based on the modified structureless pseudopotential formalism. The results obtained for Fermi energy of undeformed metals were in agreement with the experimental values which shows the validity of the model used in the computation. The electron density parameter of transition and noble metals are least affected by deformation unlike simple metals. The effect of deformation on Fermi wave vector depends not only on the electronic density parameter but on the nature of the metals. The elastic properties of metals affect the variation of the Fermi energy of metals with deformation; the chemical potential of transition and inner transition (noble) metals is mostly affected by deformation unlike the simple metals.

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# APPENDIX

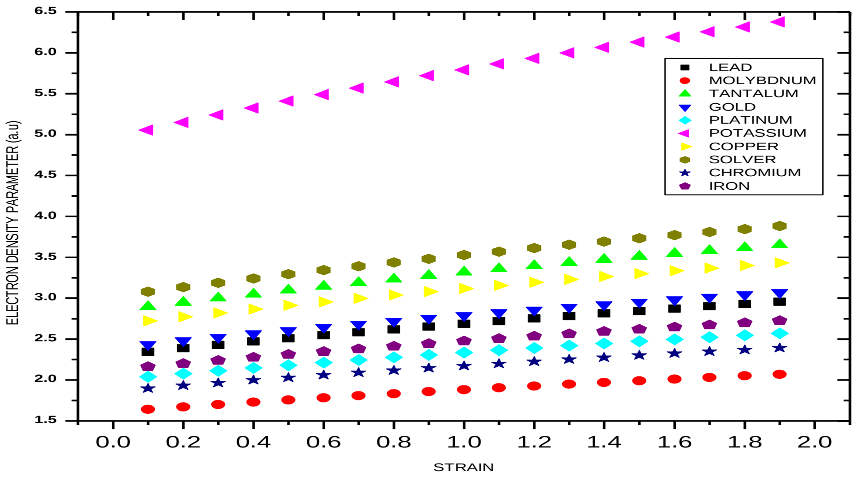

Fig .1: Variation of electron gas parameter with strain for some metals.

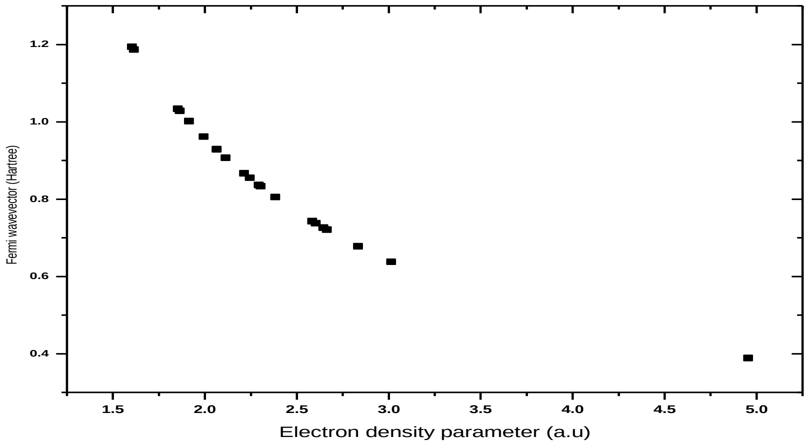

Fig.2: Variation of Fermi wavevector with electron gas parameter for some metals.

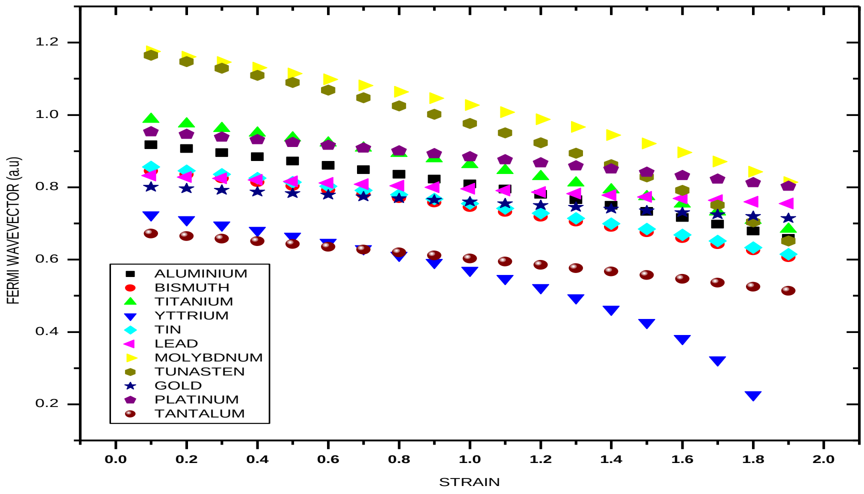

Fig.3: Variation of Fermi wavevector with deformation for some metals.

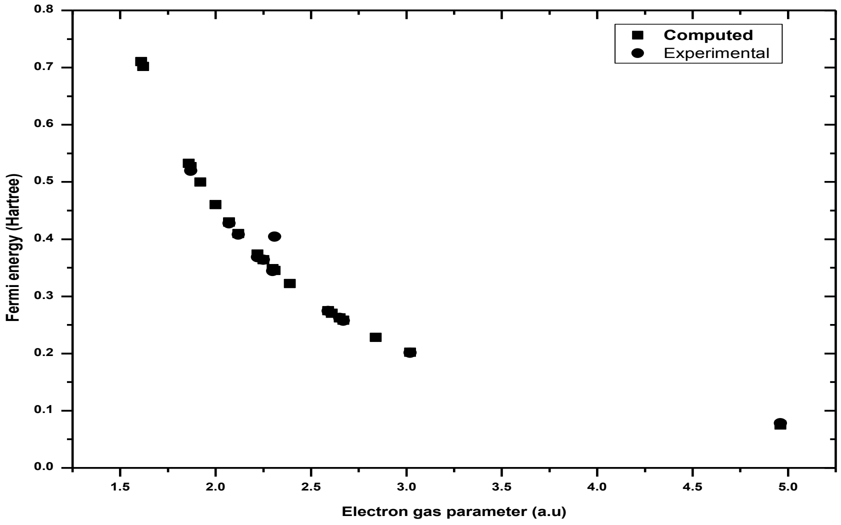

Fig.4: Variation of Fermi energy with electron gas parameter for some metals.

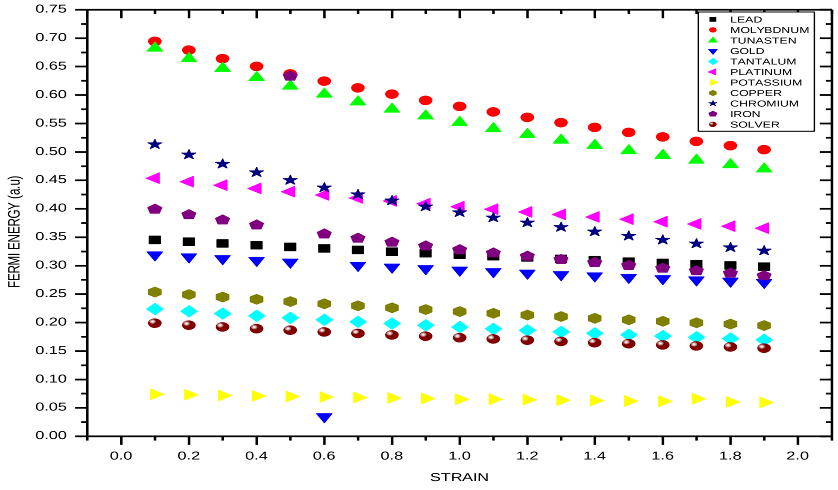

Fig. 5: Variation of Fermi energy with deformation for some metals

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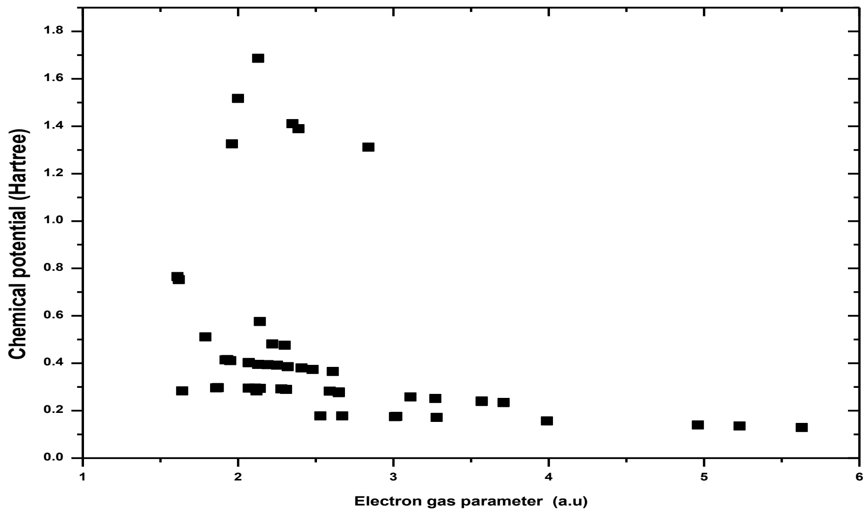

Fig.6: Variation of Chemical Potential with Electron gas Parameter for some metals.

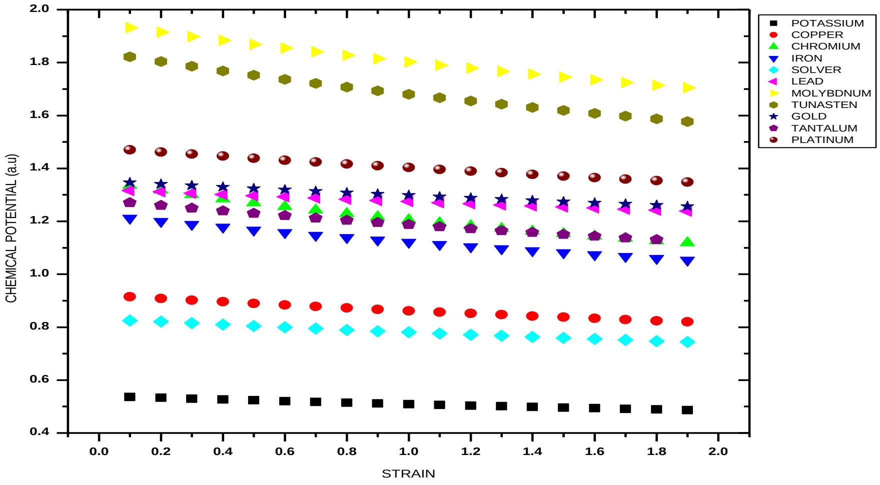

Fig. 7: Variation of Chemical Potential with Deformation for some metals.