

## EFFECT OF DEFORMATION ON THE STRUCTURAL PROPERTIES OF SOME TRANSITION METALS

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### Abstract

The structural properties of the deformed metal are of great significance in their technical and industrial applications. In this work; the structural properties of deformed transition metals were computed using the structureless pseudopotential formalism. The result obtained revealed that deformation causes an increase in the binding energy, causes a decrease in bulk modulus, an increase in compressibility ratio and causes increase in cohesive energy. The results obtained in this study for the structural properties of deformed metals showed that deformation affects the structural properties of transition metals and the success of the structureless pseudopotential formalism in predicting the properties of solids.

**Keywords:** Transition Metals, Deformation, Structureless Pseudopotential formalism, Structural properties and computing.

### INTRODUCTION

Metals are generally malleable, they can be hammered or pressed permanently out of shape without breaking or cracking and are fusible and ductile. Metals in general have high electrical conductivity, high thermal conductivity, and high density. Metals are generally not used in their pure state but as mixtures of metals or metal and non-metal constituents commonly referred to as alloys (Selman, 2015). Deformation describes how an object's shape or size changes as a result of applied forces or temperature changes. For modest enough strain or stress, all solid materials display virtually identical behaviour, so a solid body deforms when tension is applied to it. When external forces are applied to a material, its behaviour is determined by the magnitude of the forces, the material's inherent strength, and how the forces are applied and integrated. The material may deform plastically or elastically as a result of the particular mix of forces.

Knowing the intensity of the forces at all sites across the material determines the amount of deformation. (HughFord and Alexander, 1977). Torsion, tensile, and compressive forces can all deform metals, depending on the metallic surface area that is subjected to distinct deformations, atoms in the interior and those on the surface of the metals shift coupled with their atomic distance during deformation. The contact potential difference on the metal surface is also altered by deformation (Borg, 1990). Binding energy, cohesive energy, Young's modulus, Poisson's ratio, yield strength, and ultimate strength are all mechanical parameters of metal that have become important in engineering material study and design (Adeshakin, 2017). At absolute zero temperature, the cohesive energy is the amount of energy necessary to break down a given mass of solid metal into free atoms. The strength of the forces that hold atoms together in the solid state is measured by cohesive energy. It results from the interaction between the core and valence

electrons, as well as the electronic energy and electron-electron interaction energy (Adeshakin, et al., 2012). A flexible way for calculating many solid state properties is pseudopotential formalism. The pseudopotential formalism uses the valence electrons to explain the physical characteristics of atoms, molecules, and solids. It is typical to establish an effective potential between the valence electrons and the atomic core that is weaker than the true potential to avoid a difficult all-electron challenge (Osiele, 2005). Models based on pseudopotential formalism have been used to describe many phenomena in solids over time. The pseudopotential formalism, for example, is useful for describing binding energy, cohesive energy, and surface features of simple metals (Perdew et al., 1998). Vackar et al., (1998) constructed an all-electron pseudopotential and used it to determine the lattice constant and bulk modulus of silicon, diamond, cobalt, and titanium, and his results were in perfect agreement with experimental values. The crystal structure, bulk modulus, and lattice dynamics of simple metals were computed using the pseudopotential formalism and the results obtained were in good agreement with experimental values and compared very well with results obtained

using other computational methods (Pollack, et al., 1998). The self variational-consistent treatment of metal ground state properties gave rise to structureless pseudopotential formalism (Lang and Kohn, 1971). Mechanical stability is required by the structureless pseudopotential formalism, which ignores the crystal structure of metals. It has the following advantages: computational simplicity, physical transparency, fewer input parameters, and compatibility with density functional theory. The valence, core radius, and electron density parameters are the input parameters for the structureless pseudopotential. Different metallic characteristics have been computed using the structureless pseudopotential formalism (Adesakin et.al, 2012). The structureless pseudopotential formalism is extended in this work to the computation of binding energy, cohesive energy, compressibility ratio, and bulk modulus of deformed transition metals, to provide insight into how these different energies of metals vary as a result of the deformation.. The metals utilized to test the model were chosen based on the availability of their physical constants needed for computation and their technological and industrial applications.

### Theoretical Consideration

The energy functional of a system of interacting electrons is given as

$$E(n) = T_s(n) + E_{xc}(n) + \frac{1}{2} \int dr dr' \frac{n(r)n(r')}{|r-r'|} + \int dr \sum \Phi(|r - R_i|)n(r) + \frac{1}{2} \sum'_{ij} \frac{Z^2}{|R_i - R_j|} \quad (1)$$

The first three terms in equation (1) represent the kinetic energy, exchange-correlation energy and electrostatic energy, respectively. The last two refer to the Coulomb contact between ions and electrons at sites along with the pseudopotential interaction between electrons and ions. It is advantageous to add and subtract a neutralizing positive background of jellium, in order to achieve the convergence of the individual coulomb terms appearing in equation (1).

In the presence of the ionic pseudopotential, the energy functional can be written as

$$E(n) = T_s(n) + E_{xc}(n) + \frac{1}{2} \int dr \Phi([n]; r)[n(r) - n_+(r)] + \int dr \delta v(r)[n(r) - n_+(r)] + \int dr \sum_i \Phi(|r - R_i|)n_+(r) + \frac{1}{2} - \int dr dr' \frac{n_+(r)n_+(r')}{|r-r'|} - \int dr \sum_i \frac{z}{|r-R_i|} n_+(r) + \frac{1}{2} \sum_{ij} \frac{z^2}{|R_i-R_j|} \quad (2)$$

where  $\Phi([n]; r) = \int dr' \frac{n(r')-n_+(r')}{|r-r'|}$  and  $\delta v(r) = \sum_i \Phi(|r - R'_i|) + \int dr' \frac{n_+(r')}{|r-r'|}$  (3)

Only the first four terms in equation (2) depends on n(r) then equation (3) can be written as

$$E[n]=T_s[n]+E_{xc} [n]+\frac{1}{2} \int dr \Phi([n];r)[n(r)-n_+(r)]+\int dr \delta v(r)[n(r) - n_+(r)] \quad (4)$$

Equation (4) differs from jellium model by the inclusion of the last term. Thus the self – consistent electron density may be constructed from the auxiliary wave functions which satisfy Schrodinger equation.

$$[-\frac{1}{2}\nabla^2+v_{eff}(n; r)]\varphi_i(r) = E_i\varphi_i(r) \quad (5)$$

with the effective potential.

$$V_{eff}(n;r)=\Phi(n; r)+\delta v(r) + v_{xc}(n; r) \quad (6)$$

where  $v_{xc}(n; r) = \frac{\delta E_{xc}}{\delta n(r)}$

The Madelung energy of the neutralized lattice is the final term in equation (4).

As a result, the binding energy, which is the total energy needed to assemble the valence electrons and ions to form the solid is

$$E= T_s(n) + E_{xc} + W_R + E_m \quad (7)$$

where  $T_s$  is the kinetic energy,  $E_{xc}$  is the sum of the exchange and correlation energies,  $W_R$  is the average value of the non-coulombic part of the pseudopotential and  $E_m$  is the average madelung or electrostatic energy of points ions embedded in a uniform negative background of density, n.

In the low-density limit of the density functional theory, the kinetic and exchange energies are given as

$$T_s = -\frac{1.105}{r_s} \text{ and } E_x = -\frac{0.458}{r_s} \quad (8)$$

where  $E_x$  is the exchange energy and  $r_s$  is the electron density parameter

The correction energy used in the work is that Carperley and Alder (1976) as parameterized by Perdew and Zunger (1981) and is given as

$$E_c = -\frac{0.1423}{1+1.0529r_s+0.3339r_s} \quad (9)$$

In the structureless pseudopotential model, the binding energy of metal per electron is calculated using equation (7), from which we obtain

$$B.E = \frac{1.105}{r_{su}} - \frac{0.458}{r_{su}} - \frac{0.1423}{1+1.0529r_{su}^{\frac{1}{2}}+0.3339r_{su}} + W_R + E_m \quad (10)$$

In the structureless pseudopotential model,  $W_R$  is the average value of the non-coulombic part of the pseudopotential,  $W_R$  and the average madelung or electrostatic energy of points ions embedded in a uniform negative background of density,  $E_m$  are given as (Osiele and Edema, 2009)

$$E_m = \frac{9z}{10r_o} \tag{11}$$

and

$$w_R = \frac{3r_c^2}{2r_s^2} \tag{12}$$

where  $r_o = Z^{\frac{1}{2}}r_s$  and Z and the valency

The binding energy in the structureless pseudopotential model can be written as

$$B.E = -\frac{1.105}{r_{su}} - \frac{0.458}{r_{su}} - \frac{0.1423}{1+1.0529r_{2su}^1 + 0.3339r_{su}} + \frac{3r_c^2}{2r_s^3} - \frac{9Z}{10r_o} \tag{13}$$

where  $r_c$  is the Ashcroft core radius obtained from the bulk stability condition given as

$$r_c = \left[ -\frac{2}{15} \left(\frac{9\pi}{4}\right) r_s^{\frac{2}{3}} + \frac{1}{6\pi} \left(\frac{9\pi}{4}\right) r_s^{\frac{1}{3}} + \frac{1}{5} Z^{\frac{2}{3}} r_s^2 + \frac{2r_s^4}{9r} \frac{dE_c}{dr_s} \right]^{\frac{1}{2}} \tag{14}$$

where  $E_c$  is the correlation energy .

Structure-preserving, volume-changing deformation is measured by the bulk modulus, which is:

$$B = -v \left( \frac{\partial P}{\partial V} \right) N = \frac{1}{12\pi} \left( \frac{1}{r_s^2} \frac{\partial^2 E}{\partial r_s^2} - \frac{2\partial E}{r_s^2 \partial r_s} \right) \tag{15}$$

where pressure, P is

$$P = - \left[ \frac{\partial E}{\partial V} \right] N = \frac{1}{4\pi r_s^2} \frac{\partial E}{\partial r_s} \tag{16}$$

The compressibility of metals at zero degrees is

$$\tau = \frac{1}{\frac{1}{12\pi} \left( \frac{1}{r_s^2} \frac{\partial^2 E}{\partial r_s^2} - \frac{2\partial E}{r_s^2 \partial r_s} \right)} \tag{17}$$

The ratio of the non-interacting electron gas to the interacting electron's compressibility as (Bowen, et al.,1994)

$$\frac{K_{free}}{K} = \left[ 1 - \frac{4}{\pi} \alpha r_s \frac{1}{4} \frac{\pi \alpha}{24} r_s^5 \frac{d}{dr_s} \left( \frac{1}{r_s^2} \frac{dE_c}{dr_s} \right) \right] \tag{18}$$

where  $r_s$  is the electron density parameter,  $\alpha = \left(\frac{4}{9\pi}\right)^{\frac{1}{3}}$  and  $E_c$  is the correlation energy per electron.

For a deformed metal, the electron density is obtained (Adeshakin et al., 2012) as

$$r_{su} = r_s [1 + (1 - 2\nu)u_{xx}] \tag{19}$$

where  $r_s$  is the electron density parameter of the undeformed metal,  $\nu$  is the poisson ratio relating the transversal compression to elongation in the direction of applied deformation and  $U_{xx}$  is the uniaxial strain, which accounts for the deforming force.

At absolute zero temperatures, the cohesive energy is the amount of energy needed to break up a given mass of solid metal into free atom. According to Elliott (1997), the net atomic energy of the Fermi gas in a deformed metal is calculated from that of undeformed metals and is written as

$$U_{fg} = \frac{2.21}{r_{su}^2} - \frac{0.916}{r_{su}} - (0.115 - 0.0313 \ln r_{su}) \tag{20}$$

The inter – electron repulsion within the cell is

$$U_{ws} = U_{ei} + U_{ee} \tag{21}$$

where  $U_{ei}$  is electron –ion attractive interaction given (Elliott, 1997) as

$$U_{ei} = \frac{-3Z^2 e^2}{8\pi \epsilon_0 r_{su}} \left[ 1 - \left( \frac{r_c}{r_{su}} \right)^2 \right] \quad (22)$$

And  $U_{ee}$  is the electron-electron attractive interaction given as

$$U_{ee} = \frac{3Z^2 e^2}{20\pi \epsilon_0 r_{su}} \quad (23)$$

Hence ;

$$U_{ws} = \frac{-3Z^2 e^2}{8\pi \epsilon_0 r_{su}} + \frac{3Z^2 e^2}{20\pi \epsilon_0 r_{su}} \quad (24)$$

The cohesive energy is expressed in its entirety as

$$U_{coh} = ZU_{fg} + U_{ws} \quad (25)$$

where  $Z$  is valency.

The cohesive energy of deformed metals in atomic units can be expressed as

$$U_{coh} = Z \left[ \frac{2.21}{r_{su}^2} - \frac{0.916}{r_{su}} - (0.115 - 0.0313 \ln r_{su}) \right] - \frac{3Z^2}{r_{su}} \left[ 1 - \left( \frac{r_c}{r_{su}} \right)^2 \right] + \frac{1.2Z^2}{r_{su}} \quad (26)$$

In computing the properties of deformed metals, we first compute the electron density parameter of the deformed metal using the electron density parameter of the undeformed metal. The electron density parameter  $r_{su}$  of the deformed metal is now used in place of electron density parameter of the undeformed metal,  $r_s$  to compute the required property of the deformed metal.

### Results and Discussion

Fig.1 shows the variation of the computed binding energy with strain. The graph shows that increase in strain causes an increase in the binding energy of the metals, The figure reveals that as strain increases, the binding energy of molybdenum, tungsten, tin and lead increases. The binding energy of titanium and yttrium though their values are higher than that of others do not vary significantly with strain. This observed trend shows that the stronger the mechanical strength of a metal is the less the effect of strain on its binding energy. This may due to the fact that the applied deformation causes an increase in inter-atomic spacing in the metals. Also, deformation (or strain) causes a decrease in the interactions between the electrons in the metals. (Adeshakin et al., 2012). Fig.2 shows the variation of bulk modulus with strain for some transition metals. The figure reveals that as strain increases, bulk modulus of these transition metals decreases. This may be due to an increase in fracture density, or a rise in

pressure during deformation because bulk modulus measures the volume changing deformation (Kittel, 1996) The rate of decrease of bulk modulus with strain is higher in Molybdenum followed by Tungsten and least in Yttrium. This seems to suggest that the more tightly bond the atoms in a metal are, the greater the effect of strain on its bulk modulus. Tin and lead have very similar variation of their bulk modulus this may be due to their similar properties like valence and the similar electronic concentration which affected the computed bulk modulus. Fig .3 shows the variation of compressibility ratio with strain for transition metals. As shows in the figure above, the compressibility increases with an increase in strain .The figure reveals that Yttrium has the highest increase in compressibility ratio with strain followed by lead while tungsten and molybdenum are the least. This shows that the least strongly bond the atoms in a metal is, the more likely its compressibility ratio will be affected by strain since strain causes an increase in the inter

particle spacing of the metals. Fig. 4 shows the variation of cohesive energy with strain for some transition metals. As show in the figure, the cohesive energy of Molybdenum and tungsten increases with strain while the cohesive energy of yttrium, tin and lead does not varies significantly with strain. This shows that strain affect the cohesive energy of metals that are tightly bonded more than those that are loosely bonded. This observation could be due to the crystal structure and the inter-atomic forces acting in the metal as these affects the bonding of the atoms in the metals (Kittel, 1996).

**Conclusion**

This work have successfully shown how binding energy, bulk modulus, compressibility ratio and cohesive energy of some transition metals are affected by strain. While increase in strain causes increases in binding energy compressibility ratio and cohesive energy. Also an increase in strain causes a decrease in bulk modulus. In general, effect of strain on these structural properties of these transition metals depends on how closely packed or packing density and strength of these metals. This work has shown that structural properties of metals are affected by deformation.

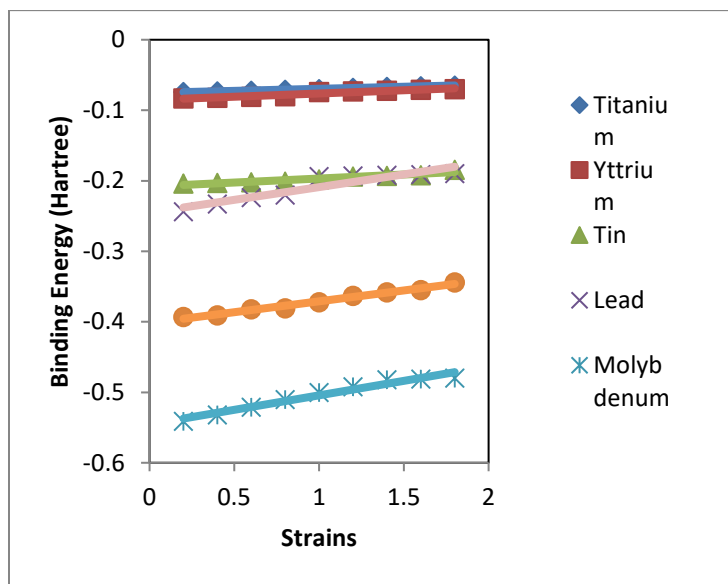


Fig 1: The variation of binding energy with deformation for some transition Metals

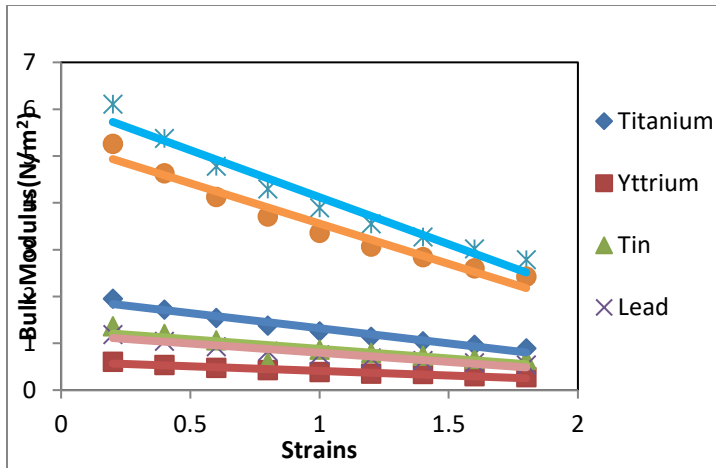


Fig.2: Variation of bulk modulus with strain for some transition metals.

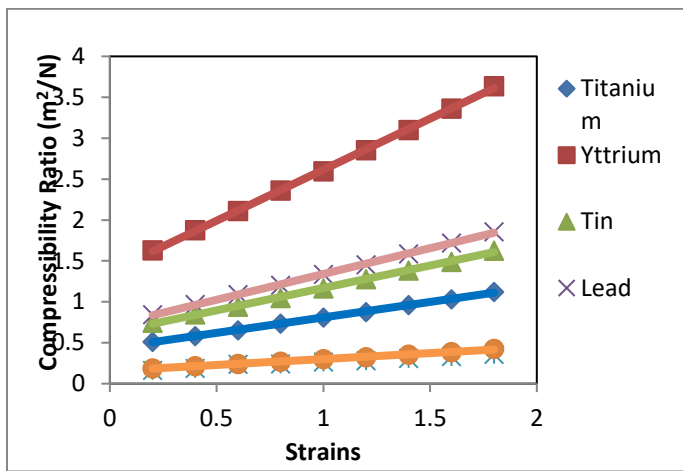


Fig.3: Variation of compressibility ratio with strain for some transition Metals

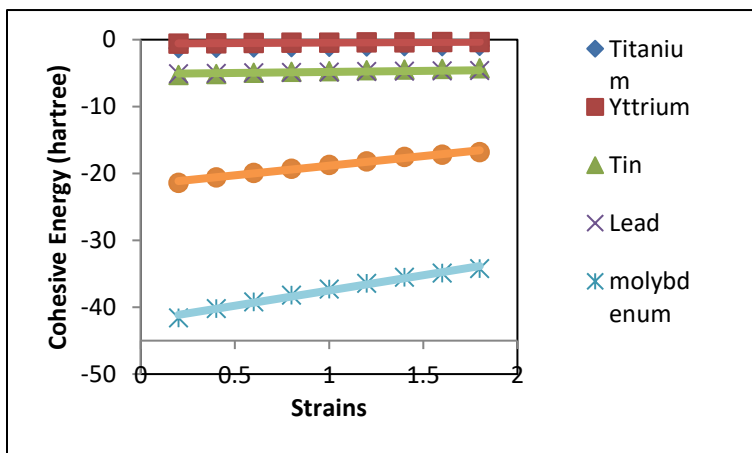


Fig 4: Variation of cohesive energy with strain for some transition Metals

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