



Effects Of Deformation On Strain Energy Density Of Metals

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Abstract: In this work, a generalized approach for computing the strain energy density of metals and the effects of deformation on it based on the structureless pseudopotential formalism is presented. The approach was used to compute the strain energy density of some metals and its variation with deformation was studied. The results obtained revealed that strain energy density of metals varies in an irregular manner with electron density parameter. Metals in the high-density limit have high values of strain energy density while metals in the low density limit have low values of strain energy density. Furthermore, the variation of strain energy density with deformation varies in different manner for different metals depending on the nature and intrinsic properties of the metals.

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1.0 Introduction

Metals achieve structural stability by letting their valence electrons roam freely through the crystal lattice. These valence electrons are the equivalents of the molecules of an ordinary gas. It is assumed that the electrons are moving about at random and colliding frequently with the residual ions (Pillai, 2010). Surface energy of solids is one of the important electronic properties of solid surfaces and controls a wide range of phenomenon such as stress for brittle fracture, the rate of sintering and the growth rate during particle coarsening. Surface energy is the energy required to create unit area of new surface and can also be described as the amount of work per unit area required to split an infinite crystal into two halves (Kiejna and Pogosov, 1999). Surface stress is the solid state analogue of surface tension. Surface stress originates from the nature of chemical bonding of atoms at the metallic surface. The atoms at the surface of an undeformed metal would have equilibrium inter atomic distance different from that of the interior atoms if the surface atoms were not constrained to remain structurally coherent with the underlying lattice (Cammarata, 1994). Atoms at the surface and interior of metals change during deformation along with their atomic distance depending on the metallic surface area that is subjected to different deformation (Sanders, 2003). Deformation is the change in the shape or size of an object during stress or strain. The study of the elastic behaviour of a solid is very important in fundamental technical research. In

technology, it tells us about the strength of the materials and 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. The elastic properties of a homogenous crystal are generally anisotropic. In a cubic crystal, the relationship between stress and strain depends on the orientation of the crystal axes relative to stress system (Kachhava, 1992). As a result of the anisotropy of crystals, 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 ϵ_{ij} , called a strain tensor which has three independent components in a system with cubic symmetry (Animalu, 1977).

The concept of strain energy is of fundamental importance in applied mechanics. The application of the stress in a metallic string produces strain. The effect of this strain is to increase the energy level of the string itself. Strain energy is stored within an elastic solid when the solid is deformed under load. In the absence of energy losses, such as from friction,

damping or yielding, the strain energy is equal to the work done on the solid by external loads. Strain energy is a type of potential energy. The energy stored in a body due to deformation is called the strain energy. The strain energy per unit volume is the strain energy density. The strain energy density at the yield point is the modulus of resilience. The strain energy density at rupture is modulus of toughness. Strain energy or strain energy density is a scalar quantity (Gavin, 2011). Consequently, a lot of efforts have been made to study the effects of deformation on some properties of selected metals. Adeshakin and Osiele (2012) developed a model for computing the surface energy and surface stress of deformed metals based on the structureless pseudo potential formalism. The developed models were tested by using them to compute the surface energy and surface stress of different classes of metals for different values of strain deformation. The results obtained revealed that deformation causes a reduction of surface energy and this reduction in surface energy is more pronounced in simple and alkaline metals. For surface stress of deformed metals, tensile stress is present in most metallic surfaces, although a few metals possess compressive stress on their surfaces. In the presence of deformation, the surface stress of some metals decreases. For Ti and Pt, deformation causes an increase in their surface stress, while deformation causes an increase in the surface stress of Mo and W causing the stress on their surfaces to change from compressive to tensile. But for Cr, Be and Al, the stress on their surfaces changes depending on the amount of deformation. 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. Keijna and Pogosov, (2000) experimentally investigated the effect of deformation on some electronic properties of metals by measuring directly a sample of deformed metals using Kelvin method. They observed that the contact potential difference of metals increase/decreases when compressed/tensed. Shore and Rose (1991), calculated the surface properties of metals based on ideal-metal model. The results of the calculated surface properties

are in agreement with experimental results but have slightly less satisfactory agreement for bulk properties than that of the structureless pseudopotential model of Perdew et al., (1990). Sarria et al., (2000), calculated the surface energy of metals based on the quantum size effects using structureless pseudopotential formalism. They found that the surface energy of metals increase rapidly at high valence electron density. Their results were in good agreement with experimental results. They also calculated the self – consistent surface energy of stabilized jellium using the local – density approximation. The results obtained were compared with those obtained for a semi – infinite stabilized jellium and were found to be in good agreement. Lang and Kohn (1971), theoretically calculated the face dependent surface properties of metals based on electron densities determined for jellium based on perturbation theory. The results obtained shows that the surface properties of metals are greatly influenced by deformation is in agreement with experimental results. Kiejna and Pogosov (1999), theoretically determined the effect of deformation on the surface properties of metal, based on stabilized jellium model, and derived modified equations for the stabilization energy of the deformed Wigner Seitz cell as a function of the bulk electron density and the given deformation. They used the electron density parameter, Poisson ratio and young's modulus of the metals as the input parameter. The results obtained were in agreement with experimental values. 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. Osiele and Edenma (2009), developed a model to compute the bulk modulus and kinetic energy contribution to the bulk modulus of metals based on structureless pseudopotential model. The computed bulk modulus of metals were in good agreement with experimental values for metal in low density limit and the agreement between the computed and experimental bulk modulus of metals decreases towards the high density limit. The results also revealed that the kinetic energy contributes significantly to the bulk modulus of metals. Osiele and Olubosede (2007) developed a stabilized jellium model to compute the surface stress and face dependent surface stress of metals. The surface stress of metals, computed using the stabilized jellium model, was compared with results obtained using other methods and available experimental values. The results obtained revealed that tensile stress

is present on the surfaces of the metals, and metals in the high density limit have high strain derivative and high values of surface stress while metals in the low density limit have low strain derivatives and low values of surface stress. Mahan (1975) calculated the variational surface energy of the jellium model of a metal surface. He used variational parameters which only affect the surface properties of the wave functions. He obtained the kinetic, electrostatic and exchange energies of metals using these wave functions. The results were compared with that of Lang and Kohn (1971) and it was found to be in good agreement. Sarria et al., (2000) investigated the quantum size effects on the surface energy the density yielding energy stability of metals, by examining the thin films of two simple metals (aluminium and lithium) in the stabilized jellium model. And found that the stabilized jellium model predicts positive surface energies that increase rapidly at high electron densities as shown by experiment while the, jellium model predicts surface energies that are strongly negative at these densities. Wojciechowski (1995) calculated the bulk properties of the stabilized uniform interstitial electron gas in metals. He employ the stabilized – jellium model and the use of the bonding – valence and interstitial – density parameters. The results obtained are quite in good agreement with available experimental values.

Brajczewska et al., (2001) calculated the dependence of metals surface properties on the valence – electron density in the stabilized jellium model whose valence electron density is described by the density parameter is as its single input. The results obtained were quite in good agreement with available experimental results. Skriver and Rosengaard (1992) calculated the surface energy for six close – packed surfaces of metals based on the linear muffin – tin – orbital’s method within the tight – binding and atomic sphere approximations. The results of the surface energy obtained are in excellent agreement with available experimental values.

In this work the structureless pseudopotential is extended to the study of the effects of deformation on the strain energy density of some metals. This will provide an insight into how the strain energy density of metals changes with deformation. The metals were chosen based on their technological and industrial applications and availability of some physical constants that are required for computation.

2.0 Theoretical Consideration

For a metal under the action of a deforming force, the average electron density in such a metal as a function of deformation is expressed as (Pogosov and Shtepa, 2006).

$$n = n_0 \left[1 - (1 - 2\nu) u_{xx} \right] + 0 u_{xx}^2 \quad (1)$$

where ν is the Poisson ratio relating compression to elongation in the direction of applied deformation, u_{xx} is the applied deformation or strain and n_0 is the average electron density in the bulk of undeformed metal and is given as $n_0 = 3/4\pi r_s^3$ and r_s is the electron density parameter of undeformed metal. For a metal under the action of a strain or deforming force, the electron density parameter of the metal is (Adeshakin, 2013)

$$r_{su} = r_s \left[1 + (1 - 2\nu) u_{xx} \right]^{1/2} \quad (2)$$

For an elastic material that is being deformed, the strain tensor is

$$\varepsilon_{ij} = \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) / 2 \quad (3)$$

Equation (3) is convenient for calculations but its disadvantage is that linear constitutive equations can only be used if the solid experiences small rotations as well as small changes in shape.

The strain can be separated into the elastic strain and thermal strain.

$$\varepsilon_{ij} = \varepsilon_{ij}^e + \varepsilon_{ij}^T \quad (4)$$

where ε_{ij}^T is the thermal strain and the elastic strain is

$$\varepsilon_{ij}^e = \frac{1 + \nu}{E} \sigma_{ij} - \frac{\nu}{E} \sigma_{kk} \delta_{ij} \quad (5)$$

where E is the Young’s Modulus, ν is Poisson ratio, σ is stress tensor and δ is Kronecker delta. The strain energy density is

$$U = \int_0^{\varepsilon} \sigma d\varepsilon = \int_0^{\varepsilon} E \varepsilon d\varepsilon = \frac{E \varepsilon^2}{2} = \frac{\sigma E}{2} \quad (6)$$

This can be written as

$$U = \frac{1 + \nu}{2 E} \sigma_{ij}^2 - \frac{\nu}{2 E} \sigma_{kk} \delta_{ij} \quad (7)$$

where

$$\varepsilon_{ij}^e = \frac{\partial U}{\partial \sigma_{ij}} \quad (8)$$

and

$$\sigma_{ij} = \frac{\partial U}{\partial \varepsilon_{ij}} \quad (9)$$

Based on the work of Needs and Godfrey (1990), the surface stress can be written as

$$\sigma = \gamma(n) - \frac{n d\gamma(n)}{dn} \quad (10)$$

where $\gamma(n)$ is the surface energy and $n = 3/4\pi r_s^3$ and r_s is the electron density parameter.

The second term in the right hand of equation (10) is the strain derivative of the surface energy which in terms of r_{su} for a deformed metal can be written as (Needs and Geoffrey, 1990)

$$-\frac{n d\gamma}{dn} = \frac{r_{su}}{3} \frac{d\gamma}{dr_{su}} \quad (11)$$

Hence

$$\sigma = \gamma + \frac{r_{su}}{3} \frac{d\gamma}{dr_{su}} \quad (12)$$

Combining equations (6) and (12), we obtain the expression for computing the strain energy of deformed metals according to the structureless pseudopotential model as

$$D = \frac{1}{2 E} \left[\gamma + \frac{r_{su}}{3} \frac{d\gamma}{dr_{su}} \right]^2 \quad (13)$$

In this work, the surface energy was computed based in the parameterized expression of Brajczewska et al., (2001).

In this work, the strain energy density of deformed metals will be computed and how deformation affects this property of metals will be studied. Also the variation of strain energy density with electron density parameters will be investigated.

3.0 Results and Discussion

Figure 1 shows the variation of strain energy density with electron density parameter for some elemental metals. Fig.1 revealed that strain energy density does not exhibit a regular pattern with electron density parameter. As revealed in the figure, metals in the high density limit have high strain energy density and this decrease towards the low –density limit. This

may be due to the dependence of the strain energy on the relative location of the particles or electrons in the metals. Also, the observed trend may be due to the increase in the volume of the metals from the high density limit to the low-density limit.

Figures 2, 3, 4 and 5 shows the variation of strain energy density with deformation for metals of different valencies. Fig. 2 reveals that for deformed monovalent metals, the strain energy density of potassium is least followed by that of silver and copper. The strain energy density of potassium, silver and copper decreases with increase in deformation. This also true for zinc and cadmium in Fig.3, Yttrium bismuth and titanium in Fig. 4. Furthermore, the strain energy density of the polyvalent metals (metals whose valency is grater than three) decreases with increase in deformation. The decrease in the strain energy density

of the metals with increase in deformation may be a consequence of increase in volume of the metals as a result of the applied deformation. This further reveals that deformation causes a relative large displacement of the particles in the metals. The displacement of the particles of the metals also depends on the nature of the metals.

In Fig.2, the strain energy density of chromium increases with increase in deformation, gets to a maximum value, and starts decreasing. The same behaviour is exhibited by beryllium in Fig. 3 and titanium in Fig. 4. The behaviour of these metals may be due to the fact that the respective volume of these metals decreases as the deformation increases gets to a certain value and starts decreasing after relaxation of the metal. This may also be due to the resilience of these metals which accounts for the ability of the metals to absorb energy within the elastic limit. Also in Fig.2, the strain energy density of cadmium and nickel increases up to when the deformation is 0.6 and starts decreasing. The same behaviour is exhibited by aluminium in Fig. 4. This behaviour may be due to the ability of the metals to absorb energy without fracturing.

Generally, for the metals used to test the model, the variation of strain energy density with deformation do not exhibit a general trend. This may be due the dependence of strain energy density on the elastic properties of the metals through the Young's modulus, the type of stress present in the metals, the electronic

packing density and the type of bonding between the electrons in the metals.

This work is more general and accurate than the work of Kiejna and Pogosov (2000) that computed the surface energy, work function, strain derivative and surface stress for deformed aluminium and lithium at the (100) and (111) faces. The computation of Kiejna and Pogosov (2000) was based on the assumption that the electron density parameters of deformed and undeformed metals are equal, thereby neglecting dilation and uniaxial strain. They also assumed a Poisson ratio of 0.5 for all the metals, which is an upper limit of Poisson ratio of metals.

In our computation, Poisson ratio of different metals used in the work was obtained from Gere and Timoshenko, 1998. Uniaxial strain was obtained in our computation and used to obtain accurate values of electron density parameter of deformed metals.

4.0 Conclusion

In this work, a generalized approach for computing and studying the strain energy density of metals based on the structureless pseudopotential formalism is presented. The variation of strain energy density of metals with deformation do not exhibit a particular trend. The strain energy density of metals depends on some properties of metals such as its elasticity, nature of the internal stress in the metal, electronic bonding, inter-particle spacing, variation of the volume of the metal with deformation and resilience of the metals.

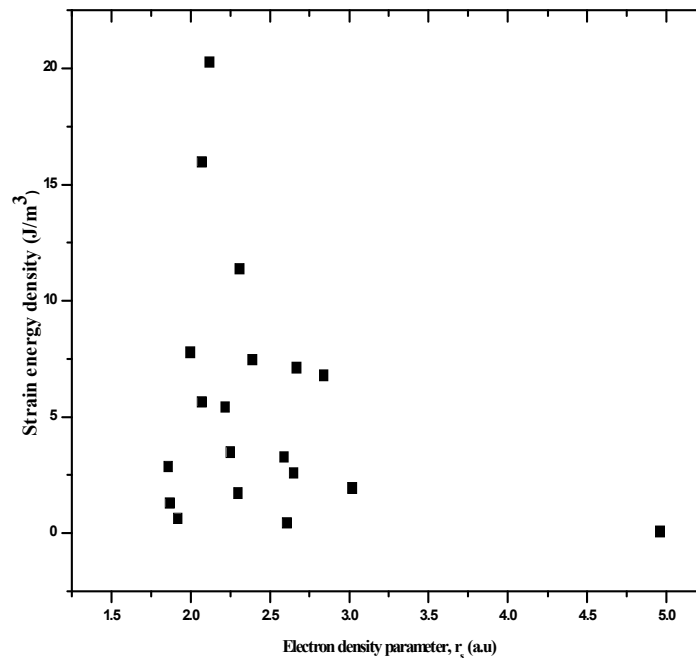


Fig. 1: Variation of strained energy density with electron density parameter for some metals.

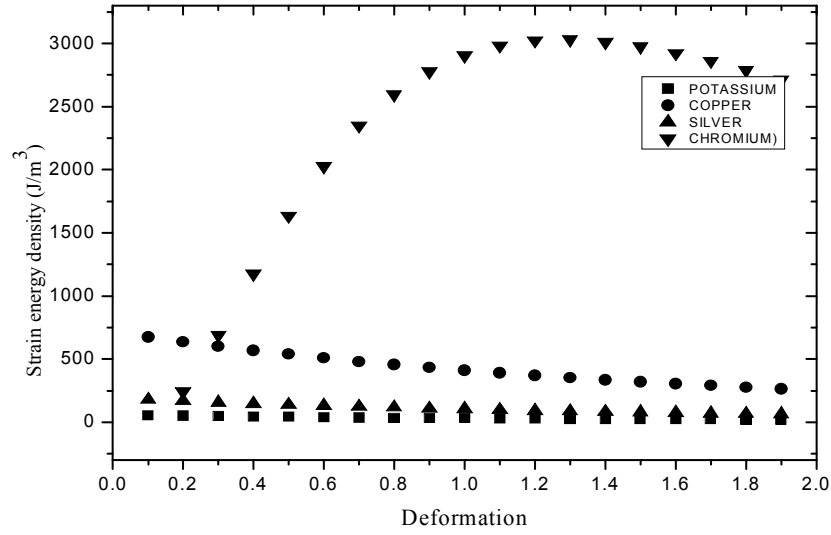


Fig. 2: Variation of strain energy density with deformation for some deformed monovalent metals.

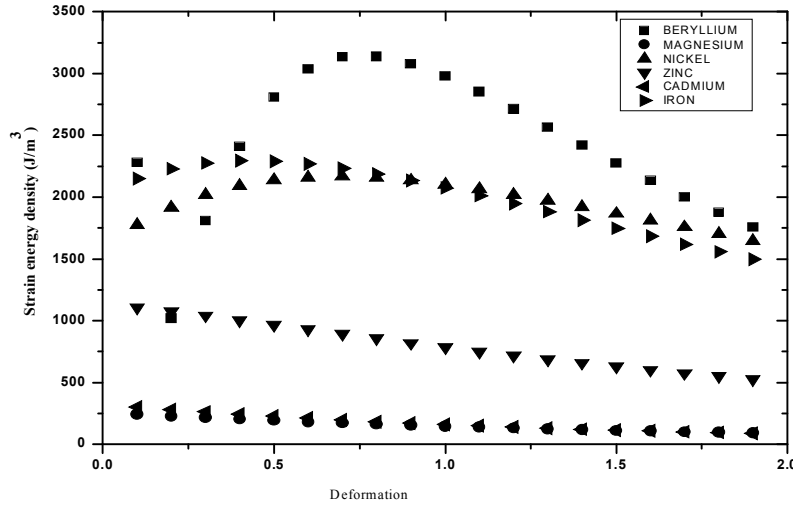


Fig. 3: Variation of strain energy density with deformation for some deformed divalent metals.

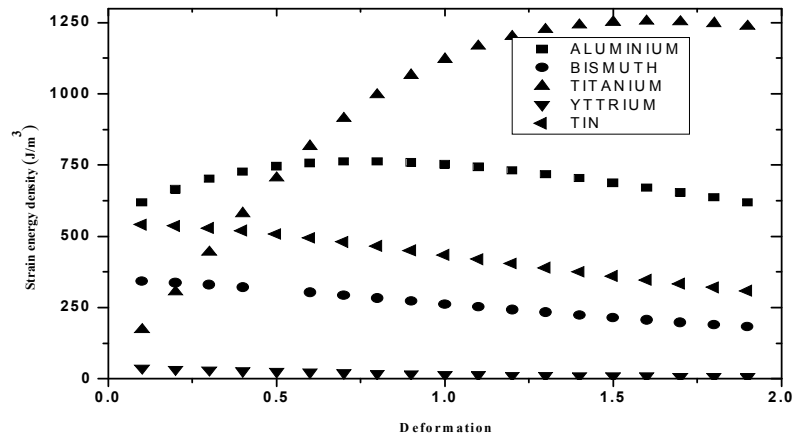


Fig. 4: Variation of strain energy density with deformation for some deformed trivalent metals.

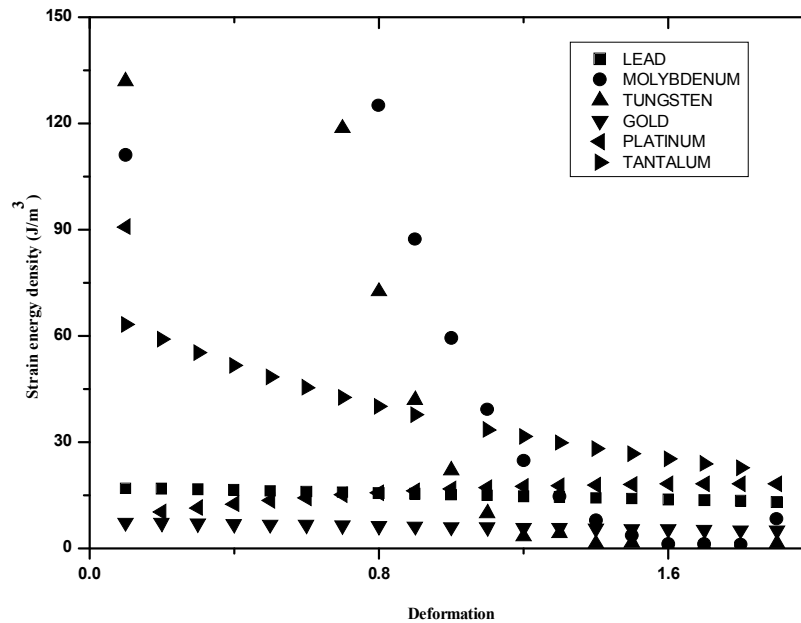


Fig. 5: Variation of strain energy density with deformation for some deformed Polyvalent metals.

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