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Theoretical Analysis of Mechanical Properties for Elements at Nano-scale

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***Abstract*— For effective product design, knowledge of material properties is essential. The measurement of material properties at nano-scale presents a challenge as its either not cost-effective or it is computation-intensive. As found in literature, for an accurate estimate of mechanical properties ultra-sonic methods in combination with particle in a box model has been employed. In this paper, we have attempted to establish a method for accurate estimates of material properties of elements based on basic physics. We have calculated the mean ultra-sonic velocity at nano-scale for Al, Au and Ag using Debye temperatures found in literature. These velocities were then used to theoretically compute and compare the mechanical properties of these elements at the bulk and nano-scales respectively. Analysis of lattice parameters at nano-scale was also performed using particle in a box model and it was found that all the three elements had a lattice contraction of 30%.**

***Keywords*— Debye temperature, lattice parameter, ultrasonic velocity**

I. Introduction

Exhaustive research in the field of nano-materials is revolutionizing fields such as medicine, manufacturing process, automobiles & aircraft industries to name few. The study of material properties is crucial to the design of a product whether it uses materials at the bulk scale or at the nano-scale. As significant changes in the mechanical properties have been found in at nano-scale, these properties are estimated either by simulations such as Molecular Dynamics or correlations as experimental measurement methods such as nano-indentation are not feasible and cost-effective.

Ultrasonic velocity is often used to estimate the mechanical properties at the nano-scale. In this paper, we have theoretically investigated the mechanical properties for Aluminium (Al), Silver (Ag) and Gold (Au) in their elemental form.

An attempt was made to estimate the ultrasonic velocity using available Debye Temperatures and hence use the estimated velocity to calculate nano-scale mechanical properties and compare with those at bulk scale. To account for the deviation of mechanical properties in nano-crystals, the lattice constant for Face-Centered Cubic (FCC) crystal of the above elements was also calculated and compared with that of the bulk crystal.

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II. Literature Review

The material properties at nano-scale have been found to be affected by the grain size and porosity. Properties such as Young's Modulus have been found to vary with porosity while yield stress is said to be affected by the grain size. Other factors such as change in deformation mechanisms at the nano-level may explain the significant differences in the mechanical properties of a material. [1]

The Debye temperature is temperature of crystal's highest normal mode of vibration, i.e. highest temperature achieved due to single normal vibration. [2] The following correlation between the sound velocity and Debye temperatures found in literature [3] has been used for our calculations.

$$\theta_D = \frac{h}{k}\left(\frac{9N_A}{4\pi V^2}\right)^{1/3}\left[\frac{2}{u_t^3}+\frac{1}{u_L^3}\right]^{-1/3} \quad (1)$$

Modeling the lattice vibrations caused by phonons as particle in box, Jozef Garai [4] has identified the limit on minimum wavelength to be equal to length of unit cell also known as lattice constant.

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Using this concept, the following equation derived has been used to estimate the lattice parameter at nano-scale.

$$\text{Lattice constant, } a = \lambda_{min} = \frac{hu_m}{k_b \theta_D} \quad (2)$$

Instead of employing computer intensive simulations for calculation of the mechanical properties, we have used the following equations from literature [3][5] to serve our purpose.

$$u_L = \left(K + \frac{4}{3}G\right)^{1/2} \rho^{-1/2} \quad (3)$$

$$u_t = G^{1/2} \rho^{-1/2} \quad (4)$$

$$E = (1 + \sigma)\, 2G \quad (5)$$

$$\sigma = [(L - 2G)/2(L - G)] \quad (6)$$

$$H = [(1 - 2\sigma)/6(1 + \sigma)]\, E \quad (7)$$

Where u_t is the transverse sound velocity, u_L is the longitudinal sound velocity, the density is ρ; the elastic constants are longitudinal modulus (L), shear modulus (G), bulk modulus (K), Young's modulus (E); Poisson's ratio (σ), Debye temperature (θ_D) and H is the microhardness. Constants found in the above equations are h which is the Plancks constant; k_B is the Boltzman constant and N_A is the Avogadro number. The molar volume V is found using, $V = M_w/\rho$ where M_w is the molecular weight.

III. Results

The Debye temperature of the nanocrystals Au, Ag, Al published in the literature [8] was used by us for our analysis to find the ultrasonic velocity as given in earlier section. This calculated velocity is then plugged into Eq. 3 to Eq. 7 specified in previous section to estimate the mechanical properties of Al, Ag, Au at nano-scale.

Upon calculation of mean ultra-sonic velocity, it was found that the Debye Temperature varies linearly with the velocity. This correlation was also observed in our theoretical analysis of doped Cadmium Oxide at the nano-scale. [6] The Fig. 1 depicts this relation for Al, Ag and Au.

The calculated velocity was used to compare mechanical properties calculated at nano-scale with those present at bulk scale. The following table 1 gives the values for the properties at nano-scale while bulk scale values were taken from online database. [7]

TABLE I

Calculated values of mechanical properties of nano Ag, Al, Au

Elements	Al	Ag	Au
Density(kg/m^3)	2700	10490	19300
Mw(10^{-3})	26.98	107.86	196.96
V(m^3)	9.99×10^{-6}	10.3×10^{-6}	10.2×10^{-6}
Debye Temp (K)	394	215	170
U_t (m/s)	2306.03	1270.42	1001.99
U_s (m/s)	2075.43	1143.37	901.79
U_m (m/s)	2340.75	1289.54	1017.07
U_L(m/s)	4612.06	2540.83	2003.97
L (Nm^{-2})	5.74×10^{10}	6.77×10^{10}	7.75×10^{10}
G (Nm^{-2})	1.16×10^{10}	1.37×10^{10}	1.57×10^{10}
K (Nm^{-2})	4.19×10^{10}	4.94×10^{10}	5.66×10^{10}
σ	0.373	0.373	0.373
E (Nm^{-2})	3.19×10^{10}	3.77×10^{10}	4.31×10^{10}
H (Nm^{-2})	0.984×10^{9}	1.16×10^{9}	1.33×10^{9}

As observed from the graphs (Fig. 2 and Fig. 3), there is significant decrease in the elastic moduli for all three elements. This decrease may be due to the reduction in grain size as suggested by literature.

The estimated values of λmin which is also the lattice parameter for the crystal at nano-scale have been compared with the edge length of the crystals. The atomic radius has been taken from Callister's textbook for materials science.

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[9]The lattice contraction was found to be about 30% as observed in Table II.

Table II

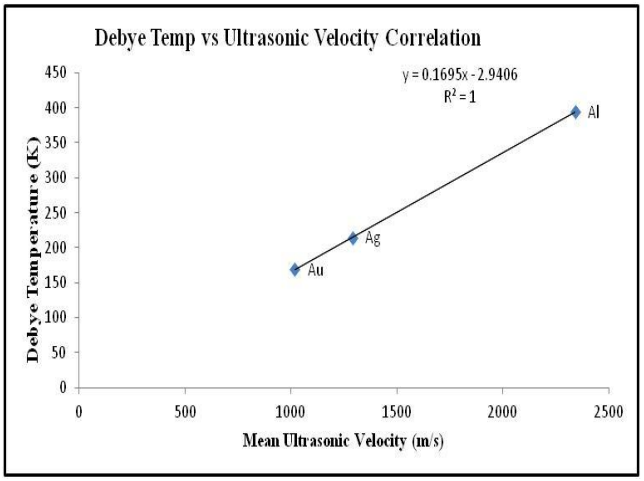
Lattice parameter calculations for nano Al, Au, Ag

Elements	Al	Ag	Au
Atomic Radius(m)	1.43E-10	1.44E-10	1.44E-10
Lattice constant (m)	4.04E-10	4.07E-10	4.07E-10
Wavelength (m) or Lattice constant at nano-scale	2.85E-10	2.88E-10	2.87E-10
Lattice contraction	-29%	-29%	-29%

IV. ONCLUSIONS

From the graph we see that the ultrasonic velocity and θD plot shows a linear relationship for Au , Ag , Al. This correlation has also been observed for theoretical analysis of doped nano-crystalline Cadmium Oxide. Further investigations are proposed for a set of materials to help in establishing a correlation between Debye Temperature and ultrasonic velocity so that Debye temperature can be established using ultrasonic methods for wide variety of materials.

Figure 1: Debye Temperature vs ultra-sonic velocity correlation for Al, Ag, Au



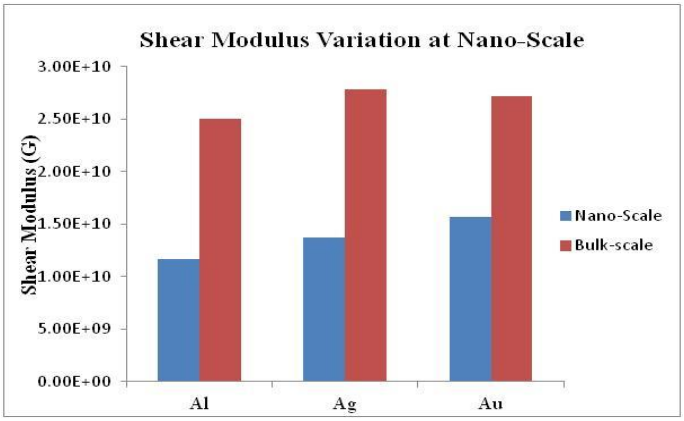


Figure 2: Shear Modulus Variations at nano & bulk scale

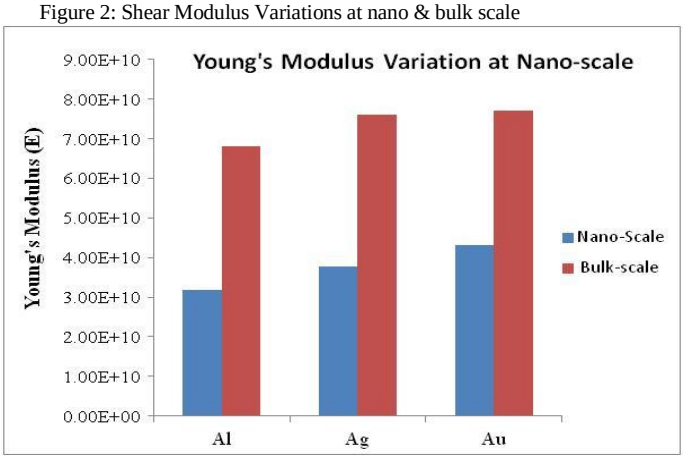


Figure 3: Shear Modulus Variations at nano & bulk scale

The elastic modulus has shown a significant decrease in their values. Though this decrease has often been attributed to grain size reduction and changes in deformation mechanism at nano-scale, these results need to be verified by simulations or experimental measurements for supportive evidence. The lattice contraction was found to be consistently 30% for all three elements. We can safely conclude that if crystals have same structure and similar atomic radii, an estimate of lattice contraction at nano-scale can made based on calculations for any one of the similar elements. In order to establish the use of ultrasonic velocity as conclusive means of determining nano-material properties, few of the calculated values have been proposed to be corroborated using experimental methods such as nano-indentation.

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