Size and Structure Dependence of the Anomalous Bulk Modulus for FCC Metallic Nanoparticles

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The purpose of this work is to develop a theoretical model to calculate the bulk moduli of FCC nanoparticles that account for their size and structure. The bulk modulus for spherical nanoparticles has been derived from the cohesive energy which had been calculated by summing up the potential energy function of every pair of atoms of these metallic nanoparticles. The *ab initio* pair potential energy function has been formed by inverting the cohesive energy function proposed by (Rose *et al*., 1981), using the Chen-Mobius method. The results show that, as the size decreases, the bulk modulus decreases for spherical nanoparticles, which agrees with previous experimental and theoretical predictions. The results also predicted an "amorphous" structure for ultra-small nanoparticles and were consistent with previous experimental work.

Keywords: *ab init*io calculations; metals; nanoparticles; bulk modulus; amorphous structure.

1 Introduction

At present, there is no internationally accepted definition of nanoparticles. However, it is quite common to define nanoparticles as objects with diameters in the range of 1-100 nm. Consequently, nanoparticles are comprised of a number of atoms from few to few thousands. At the Nano-scale level, the bulk modulus of nanoparticles shows inconsistent trends for different materials. For example, the bulk modulus is enhanced as the size decreases for some nanomaterials, such as, γ-Fe_2O_3[1], CeO_2[2], Au[3] and Ag[3] and diamond[4]. On the other hand, the bulk modulus decreases for some other nano materials, such as, γ-Al_2O_3[5], $CdSe$[6] and PbS[7]. For Nickel, the bulk modulus does not show appreciable size dependence[8,9]. The authors concluded that the bulk modulus of nickel nanoparticles is unchanged from its bulk value.

Theoretical predictions conducted by G. Ouyang *et al.*, had shown an enhancement of the bulk modulus of Ag[10]. On the contrary, Tbarakat predicted a decrease in the bulk modulus of Mo and W spherical nanoparticles as their sizes decrease[11].

The modulus as well as many other physical properties of matter can be found from the cohesive energy. Over the last two decades, many researchers tried to build physically acceptable potential energy functions (PEF) and models, and to find out the nature of atom-atom interactions within a nanoparticle[12-27], or nanotubes[28-30]. Semi-empirical PEFs with adjustable parameters have been worked out by many researchers[19,25,26]. However, a parameter-free functional pair potential has not been reported in the literature[31].

A.E. Carlsson, GelattJr, and H. Ehrenreich (CGE) were the first to introduce the inversion relation between the cohesive energy and the pair potential energy function[31]. In other words, if the cohesive energy as a function of the interatomic separation is determined, it is possible to find the pair potential function[32]. The cohesive energy is calculated then by summing up the energy of all pairs of atoms within a bulk or a nanoparticle. The CGE methodology generates a slowly converging series. Unless supercomputing machines are employed, CGE cannot be used with slowly converging potential functions, like Rose's[33,34]. It is not possible to truncate the summation after a certain number of terms of the series for slowly converging potential functions.

As an alternative to the CGE method, Nan-Xian Chen used another technique to invert the cohesive energy function[35]. He generalized the Mobius inversion formula in number-theory and was able to apply his method to multidimensional inverse lattice problems with all three kinds of cubic lattice structures (FCC, BCC and SC). The remarkable

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modification that was introduced by Chen to the CGE method generates a faster converging series that allows cutting the summation at 10-20 terms without losing the accuracy of the calculation of the cohesive energy[35].

In this paper, the cohesive energy function proposed by Rose *et al.*[33,34], which was successful to predict the bulk cohesive energy and many other thermo dynamical properties, has been tested and modified for nanoparticles. The potential energy functions of bulk materials was used by many researchers to calculate the cohesive energy and other properties of nanoparticles[14,36,37]. Chang Q Sun *et al.* used the well-known Lennard-Jonnes PEF to predict the cohesive energy for molybdenum and tungsten[14]. The Sutton-Chen potential is a many-body function that was suggested to represent the delocalized metallic bulk bonding. This Sutton-Chen PEF was used by Joswig *et al.* to calculate the total energy of aluminum clusters that include upto 58 atoms[36]. In addition, the variable-charge electrostatic plus potential (ES+) was developed for bulk properties calculation[37]. SamanAlavi *et al.* used molecular dynamics simulation for the prediction of the melting temperature of aluminum nanoparticles by employing ES+ PEF[37]. Using Rose *et al.* PEF in this work is assumed to predict the correct cohesive energy and modulus of FCC transition metals due to two main reasons. First, the bonds are metallic for the current work as well as for Rose *et al.* Reducing the size from bulk to nanoparticles is not expected to change the nature of atom-atom interaction. Second, the difference between bulk and nano properties calculations is the size which will be taken into account in running the summations over all pairs of atoms. The cohesive energy has been used to calculate the bulk modulus. Section Two of this paper explains in brief the procedure of finding the pair potential via the Chen-Mobius method and shows how the cohesive energy for bulk material is calculated. Section Three explains the model that has been used to calculate the bulk modulus in detail and applies the method to spherical nanoparticles with examples for the calculation of the moduli of gold, silver and nickel nanoparticles.

2 Methods of Calculation

In the present work, the Chen-Mobius technique has been used to calculate the cohesive energy and the bulk moduli of Au, Ag and Ni metallic nanoparticles using the pair potential energy function(PEF) suggested by J. H. Rose *et al*[33]. The calculations have

been conducted at $T = 0\,K$ for convenience and simplicity, since the difference in the cohesive energy between the absolute zero and the melting point does not exceed 5%[38].

The potential energy of N interacting atoms (at rest, $T = 0\,K$) can be written as a many-body expansion:

$$E = E_2 + E_3 + \cdots E_N \qquad \text{... (1)}$$

Explicitly,

$$E = \frac{1}{2!}\sum_{\substack{i,j \\ i \neq j}}^{N} \phi[\vec{r_i}, \vec{r_j}] + \frac{1}{3!}\sum_{\substack{i,j,k \\ i \neq j \neq k}}^{N} \phi[\vec{r_i}, \vec{r_j}, \vec{r_k}] + \qquad \text{... (2)}$$

Where $\phi[\vec{r_i}, \vec{r_j}]$ and $\phi[\vec{r_i}, \vec{r_j}, \vec{r_k}]$ denote the two- and three-body PEFs respectively. In this series, the two body interaction E_2 is dominant. If only up to dipole-dipole interactions are considered, the total cohesive energy (at $T = 0\,K$) is given by the sum over all couples of dipoles within the particle. So, the total energy is given by:

$$E = \frac{1}{2!}\sum_{\substack{i=1 \\ i \neq j}}^{N} \sum_{j=1}^{N} \phi[r_{ij}], \qquad \text{... (3)}$$

Where r_{ij} denotes the interaction distance between i and j atoms. The crystal structures for nano-Ni, Cu, Au and Ag were reported by many researchers to be the same as that of bulk[39-42]. So their structures at the nano level are FCC.

In this work, the atoms are assumed to interact via the pair potential $\phi[r_{ij}]$ derived by Chen *et al.*[43]. The derivation is explained in detail in reference[43] and outlined in the appendix of[44]. This pair potential is expanded in terms of the cohesive energy function $E(r)$ suggested by Rose *et al.*[33] and given by:

$$\phi(r) = 2\sum_{l=1}^{\infty} \beta_l E(c_l r), \qquad \text{... (4)}$$

Where c_l is a monoatomic sequence that represents the radii of spherical shells of a FCC nanoparticle. β_l's are coefficients of series expansion that can be found from the relation:

$$\sum_{(c_l|c_k)}^{k} \beta_l\, s\left(c^{-1}\left[\frac{c_k}{c_l}\right]\right) = \delta_{k1}, \qquad \text{... (5)}$$

Where δ_{k1} is the kronecker delta. The summation of Eq. 5 runs over all the factors of c_k[42]. By determining the c_l, s_l and β_l, Eq. 4 can be used to find $\phi[r_{ij}]$ whenever $E(r)$ is chosen. The calculations of c_l, s_l and β_l are straightforward and explained in detail in the appendix of[44]. The first twenty β_l, s_l and c_l terms for FCC structure are listed in table (1). A customized code has been written to generate the atom's

coordinates for FCC crystals, the minimum cohesive energy for bulk/nanoparticles as well as the bulk modulus, and the associated nearest neighbor distances. The procedures for finding $\phi[r_{ij}]$ are explained in section 2.2.

2.1 Pair potential and cohesive energy of FCC metals

To find the pair potential $\phi(r)$, one must set the function $E(c_l r)$. In the present work, the universal cohesion equation of J. H. Rose *et al.* is used for $E(c_l r)$. Rose *et al.*[30] suggested a cohesive energy function E(r) that successfully described the behavior of many bulk metals.

This function is expressed as:

$$E(r) = -E_0(1 + r^*)e^{-r^*} \qquad \dots (6)$$

$r^* = \alpha_0 \sqrt{\dfrac{9B_0\Omega}{E_0}}\left(\dfrac{r}{d} - 1\right),$ Where Ω, d, E_0 and B_0 are the atomic volume, the nearest neighbor distance, the sublimation energy, and the bulk modulus, respectively. While α_0 equals "one" in Rose's function, in this paper, it is a fitting parameter for finding the cohesive energy at the nano level.

For FCC elements, $\Omega = \frac{1}{4}a^3$. "a" is the lattice parameter. The atomic volume can be written in terms of the nearest neighbor distance "d" as: $\Omega = \dfrac{d^3}{4(d/a)^3}$. By substituting $d/a = g$,

the inter-atomic distance is given by: $r_{ij}^* = \alpha_0 \sqrt{\dfrac{9B_0}{4g^3E_0}}\left(d^{1/2}r_{ij} - d^{3/2}\right)$. Plugging this expression for r_{ij}^* in Eq. 6, Eq. 4 can be written as:

$$\phi(r_{ij}) = -2E_0 \sum_{l=1}^{\infty}\left[\beta_l\left(1 + \alpha_0\sqrt{\dfrac{9B_0}{4g^3E_0}}(c_l d^{1/2}r_{ij} - d^{3/2})\right)e^{-\alpha_0\sqrt{\frac{9B_0}{4g^3E_0}}(c_l d^{1/2}r_{ij}-d^{3/2})}\right] \qquad \dots (7)$$

Using equation (3), the cohesive energy can be calculated by running the summation over i, j and l.

$$E = -E_0 \sum_{l=1}^{\infty}\sum_{\substack{i=1 \\ i \neq j}}^{N}\sum_{j=1}^{N}\left[\beta_l\left(1 + \alpha_0\sqrt{\dfrac{9B_0}{4g^3E_0}}(c_l d^{1/2}r_{ij} - d^{3/2})\right)e^{-\alpha_0\sqrt{\frac{9B_0}{4g^3E_0}}(c_l d^{1/2}r_{ij}-d^{3/2})}\right] \qquad \dots (8)$$

2.2 Stability

A nanoparticle is assumed stable at its minimum energy. The stability condition is: $\dfrac{\partial E}{\partial \Omega} = 0$. Since the "$\Omega$" and "$d$" are related via the relation: $\Omega = Ngd^3$, the stability condition can be written as: $\dfrac{\partial E}{\partial d} = 0$, where N is the number of atoms in the bulk/nanoparticle. Therefore, the stability condition reveals:

$$0 = \dfrac{\partial E}{\partial d} = \left(\dfrac{1}{2}\right)\left(\dfrac{9B_0\alpha_0^2}{4g^3}\right)\sum_{l=1}^{\infty}\sum_{\substack{i=1 \\ i \neq j}}^{N}\sum_{j=1}^{N}\left[\beta_l\left((c_l r_{ij} - 3d)(c_l r_{ij} - d)\right)e^{-\alpha_0\sqrt{\frac{9B_0}{4g^3E_0}}(c_l d^{1/2}r_{ij}-d^{3/2})}\right] \qquad \dots (9)$$

Upon running the summation of Eq. 9, stability is found at a certain value of "d" for every nanoparticle that includes 40 atoms and more. For ultra-small particles (less than 40 atoms), stability is lost at all values of "d", *i.e.,* Eq. 9 cannot be verified for any value of "d".

3 Results and Discussion

3.1 Cohesive energy for bulk and nanoparticles

The cohesive energy of Au, Ag and Ni bulk and nanoparticles consisting of 40-12215 are calculated using Eq. 8. The quantity (in the exponent of equation 7); $\alpha_0\sqrt{\dfrac{9B_0}{4g^3E_0}}$ is assumed constant since there is a mutual simultaneous change in the nearest neighbor distance "d" as well as in α and in the mechanical properties B and E, *i.e.,* $\alpha\sqrt{\dfrac{9B}{4g^3E}}$ is equal to its corresponding bulk value $\alpha_0\sqrt{\dfrac{9B_0}{4g^3E_0}}$, at all values of N. By looking at Eq. 7, this assumption is valid since the forces within a nanoparticle are conservative, and therefore, the potential energy becomes exclusively atom-atom distance-dependent.

The summation of Eq. 8 has been run over the first 20 terms of the series, *i.e.,* l takes the values 1, 2, 3, …. 20. This summation uses the values of c_l, s_l and β_l given in table (1) and the values of E_0 and $\sqrt{\dfrac{9B_0}{4g^3E_0}}$ given in table (2).

Equation 8 predicts the bulk cohesive energy per atom for Au, Ag and Ni (FCC) elements as shown in Fig. 1.

The variation of the bulk cohesive energy of the three metals is presented, where the stable energies

Table 1 — The lattice parameters c_l, s_l, and β_l for FCC cubic structure

l	1	2	3	4	5	6	7	8	9	10
c_l^2	1	2	3	4	5	6	7	8	9	10
s_l	12	6	24	12	24	8	48	6	36	24
β_l	$\frac{1}{12}$	$\frac{-1}{24}$	$\frac{-1}{6}$	$\frac{-1}{16}$	$\frac{-1}{6}$	$\frac{1}{9}$	$\frac{1}{9}$	$\frac{1}{3}$	$\frac{1}{12}$	0
l	11	12	13	14	15	16	17	18	19	20
c_l^2	11	12	13	14	15	16	17	18	19	20
s_l	24	24	72	0	48	12	48	30	72	24
β_l	$\frac{-1}{6}$	$\frac{7}{72}$	$\frac{-1}{2}$	$\frac{1}{3}$	$\frac{-1}{64}$	$\frac{-1}{3}$	$\frac{-17}{72}$	$\frac{-1}{2}$	$\frac{-1}{2}$	$\frac{5}{24}$

Table 2 — Bulk parameters of Rose's equation for Au, Ag and Ni.

Element	Atomic Diameter (Å)	Lattice Parameter "a"(Å)	Nearest Neighbor Distance "d" (Å)	$g=d/a$	Surface Tension (eV/ Å^2)	Shear Modulus (eV/ Å^3)	Bulk Modulus (eV/ Å^3)	Sublimation Energy (eV)	$\sqrt{\dfrac{9B}{4g^3 E_0}}$ (Å$^{-3/2}$)
Au	2.884[48]	4.08[38]	2.88[38]	0.70588	0.096875[46]	0.16218[46]	1.07625[4]	3.54889[45]	1.39285
Ag	2.989[48]	4.09[38]	2.89[38]	0.7066	0.078125[46]	0.189[46]	0.72374[4]	2.63573[45]	1.32334
Ni	2.48[45]	3.52[38]	2.49[38]	0.70739	0.1315[47]	0.47417[46]	1.12304[45]	3.93284[45]	1.34726
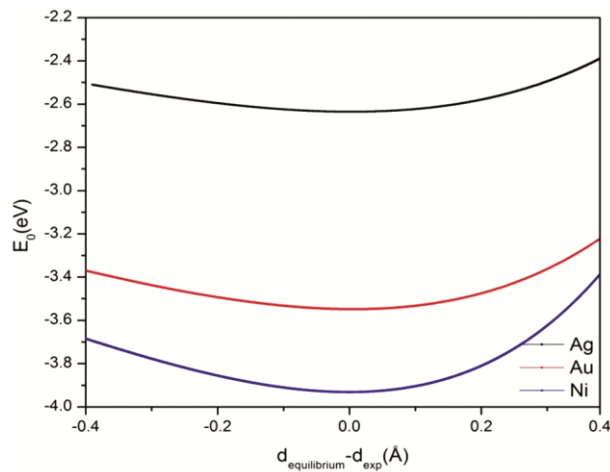
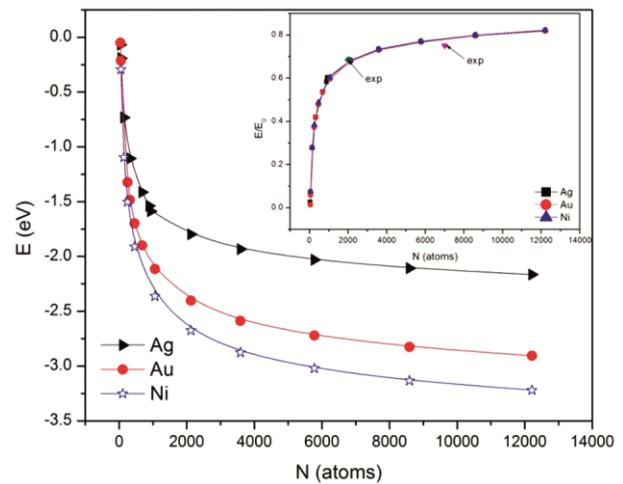Fig. 1 — The bulk cohesive energy of Au, Ag and Ni predicted by the current PEF.

Fig. 2 — The variation of the cohesive energy of Au, Ag and Ni as a function of the particle size N. The inset shows the size dependence of the scaled cohesive energy E/E_0.

(as a function of the nearest neighbor distance "d") are reached at d = 2.885Å, d =2.892Å and d =2.488 Å for Au, Ag and Ni, respectively. The cohesive energies are in agreement with the values available in the literature[45] and show that the current calculations for the energy function have an excellent agreement with the experimental predictions.

At the nano level, a nanoparticle that is comprised of N atoms is cut from a bulk FCC sample. The nanoparticles are initially assumed to have the same crystal structure as the bulk (FCC)[38-41]. As a result of cutting the nanoparticle, the constituent atoms lose stability. The atoms rearrange themselves to retrieve back the stability, and "d" is reduced as a result. It was

evident that the nanoparticles are not stable at any "d" for N less than 40 atoms. This result can be interpreted in view of amorphous structure. The nanoparticle becomes amorphous, where no equilibrium can be found at any value of the nearest neighbor distance "d". This result was predicted by H. K. Kim et al.[49].

This calculation of the cohesive energy predicted values of α different from "1". These values of α are found by fitting the experimental data to the prediction of the current work. To get the best fit for the experimental measurements, the cohesive energies for different values of "α_0" are calculated for Au, Ag and Ni, as shown in Fig. 2.

The scaled cohesive energies (E/E_0) were compared with the predictions of H. K. Kim *et al.* for molybdenum and tungsten, since they were reported to have FCC-structure at the nano level (inset of figure 2)[49]. The inset figure shows the scaled curves that collapse into almost one. Figure 2 shows the cohesive energy curves as a function of size N, where the best fit reveals "α_0" values of 0.40, 0.42 and 0.52 for Au, Ag and Ni, respectively[45].

3.2 Bulk modulus for spherical nanoparticles

The bulk modulus B is related to the cohesive energy E via the relation: $B = \Omega \frac{\partial^2 E}{\partial \Omega^2}$. This relation can also be written as: $B = \frac{1}{9gd} \frac{\partial^2 E}{\partial d^2}$ (for FCC structure). Using the expression for the energy (equation 8), B can be written as:

$$B = -\left(\frac{1}{9gd}\right)\left(\frac{9B_0\alpha_0{}^2}{4g^3E_0}\right)\left(-\frac{1}{2}E_0\right)\sum_{l=1}^{\infty}\sum_{\substack{i=1\\i\neq j}}^{N}\sum_{j=1}^{N}\beta_l\left[3\left(c_lr_{ij} - \text{d}\right) + \left(c_lr_{ij} - 3\text{d}\right) + \frac{\alpha_0}{2}\sqrt{\frac{9B_0}{4g^3E_0}}\left(c_lr_{ij} - 3\text{d}\right)\left(c_lr_{ij} - \text{d}\right)\left(c_l\text{d}^{-1/2}r_{ij} - \text{d}^{1/2}\right)\right]e^{-\alpha_0\sqrt{\frac{9B_0}{4g^3E_0}}\left(c_l\text{d}^{1/2}r_{ij} - \text{d}^{3/2}\right)}$$

$$\dots (10)$$

As has been done with calculating B, the summation[10] is run for different values of N(at the equilibrium value of "d"). The calculated bulk modulus for spherical Au, Ag and Ni nanoparticles is shown in Fig. 3. It is clear that B decreases as N decreases. Q F Gu *et al.* predicted a modulus of 1.7875-1.8125 eV/m^3 for Au (30 nm in diameter)[3]. They found also a value of .756-.868 eV/m^3 for Ag (10 nm in diameter). Compared to the values for the sizes mentioned (Fig. 3), the values of 0.46 eV/m^3 and0.875 eV/m^3 are for Au and Ag, respectively. These deviations are attributed to shape factor as well as to the very small sizes of the samples of QF Gu *et al.*[3].

A better comparison can be found by comparing the current findings to previous predictions for transition metals[11], where Tbarakat predicted similar results using Mie-type two-body plus Tellar-Axilord many-body PEFs to calculate the bulk modulus of Mo and W spherical nanoparticles Fig. 4[11].

It is clear that this model and the PEF used in this work predict the size dependence of B as well as E for spherical nanoparticles. B decreases slowly upon
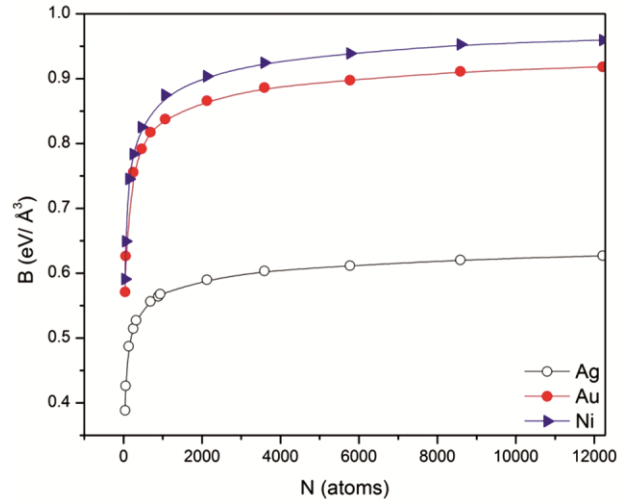

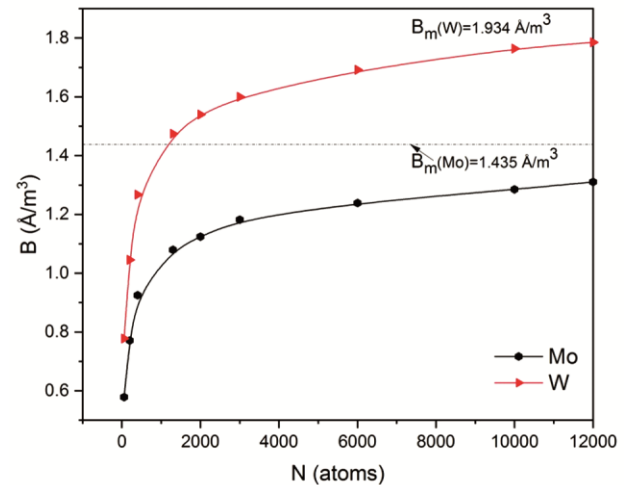Fig. 3 — The size dependence of the bulk modulus of spherical nanoparticles using the modified Rose PEF(Eq. 8).

Fig. 4 — The size dependence of the bulk modulus of FCC spherical nanoparticles of Mo and W predicted by Tbarakat[10].

decreasing the particles' size till N approaches 2000 atoms, after which it decreases very rapidly.

4 Conclusion

In conclusion, the present work shows that the modified Rose energy function predicted the correct experimental behavior of the moduli of Au, Ag and Ni spherical nanoparticles. It also shows that this potential energy function used here fits exactly the bulk measurements of the experimental cohesive energy of Au, Ag and Ni metals. Controlling the size of a nanoparticle will enable researchers to control the physical properties of nanoparticles. This will open the door for researchers to a variety of practical applications that can make use of this phenomenon.

The current results can be further used to predict other mechanical properties of elements of other structures and composite materials. This work is a step forward towards controlling the mechanical, electrical, magnetic and optical properties of nano materials.

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