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First-Principles Molecular Mechanics Calculations of the Lattice Constant and Bulk Modulus for Au-Cu Nano-Alloy

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Abstract: ***The unique mechanical properties of nanoparticles orNano alloys allow for novel applications in wide fields. In this paper, we calculate the mechanical properties of nanoparticles. We performed atomistic simulations to study the structure and Elastic constants for Au-Cu Nano-Alloy. We used approaches to compute the bulk modulus and lattice constant, one based on a definition in terms of the lattice parameter derivative of the total energy and another in terms of the volume derivative of the pressure often used in simulations. Both give quantitatively similar results.***

Keywords: Nano-alloy; lattice constant; bulk modulus; First principle calculation

1. Introduction

Nanoparticles or Nano-alloys are microscopic objects having at least one dimension less than 100 nm [1, 2]. When the particle size reaches the nanoscale, the crystal boundary is destroyed or the atomic density changes[2, 3]. Due to this change in physical properties, the use of nanomaterials varies considerably in many fields of science andtechnology [4, 5]. Gold-copper (Au-Cu) nanoparticles have been regarded as valuable tools in a variety of disciplines[6]such as the communications[7], renewable energy [8], molecular sensing [9], and medical imaging[10, 11].Some mechanical properties of Nano alloys, such as strain, tensor, the shear constant, the hardness and the bulk modulus will aid a lot in the proper design of particles in specific applications.This paper aims at the calculation of the mechanical properties of Au-Cu nanoparticles or Nano alloys, from the calculation of the lattice constant and bulk modulus by computational method.

Computational method [12] are usually considered as very useful complementary tools to experimental studies, for instance, of the mechanical properties [13]. Therefore, in this work, we use the first-principle calculations to predict the lattice structure and bulk modulus of Au-Cu nanoparticles (hereafter referred to as Nano-alloys) with size ~ 1 nm per Nano-alloy.These calculations were performed using Quantum espresso code[14].

2. Computational Methods

The first-principles calculations carried out in this study were based on density functional theory using the Quantum Espresso package [14] . We used the generalized gradient approximation (GGA)[15] for the exchange-correlation functional. The first-principles calculations were performed under pressure-volume and lattice parameter- total energy conditions.

The first stage concerned with the optimization of the lattice constants for Au, Cu, and Au-Cu bulk materials. For this purpose we used the full-potential code called Exciting [16]. After optimizing the lattice constants we then used the optimized lattice constants with the Atomic Simulation Environment (ASE)[17] to generate the nanoparticle with 13 atoms by employing the Wulff-construction method incorporated with ASE. The generated Au nanoparticle is shown in Figure 1. Where the cubic box (dashed lines) has a lattice defined by the atomic sites for the 13 Au atoms nanoparticle placed in a corner of large empty box with a side a ~ 10 Å.

The structures energies were calculated using the first-principle Quantum Espresso [14] , the uniform grid k-points were $(2 \times 2 \times 2)$.

The total energy calculations and lattice parameter were performed using density functional theory (DFT) as implemented in the Quantum espresso code [18].

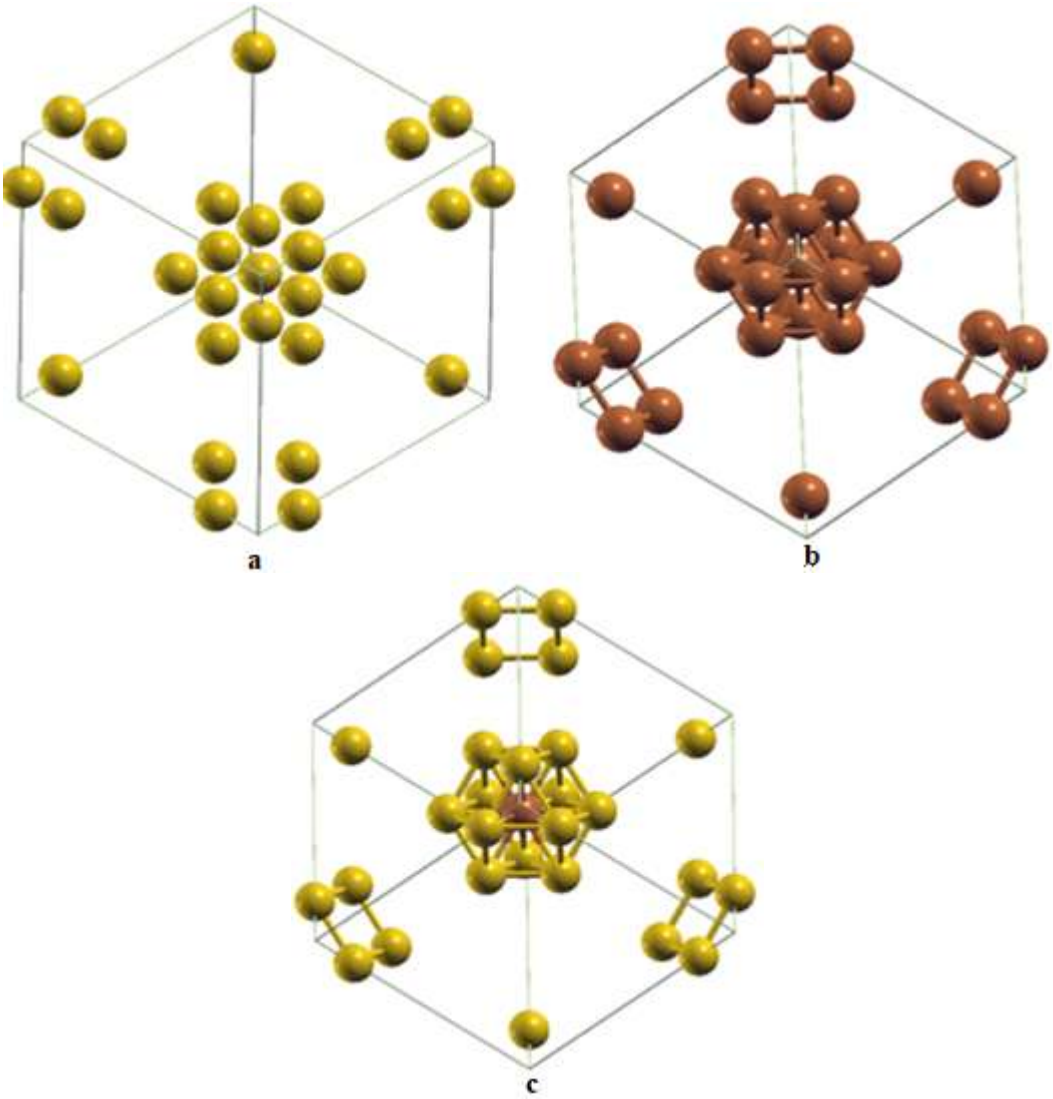
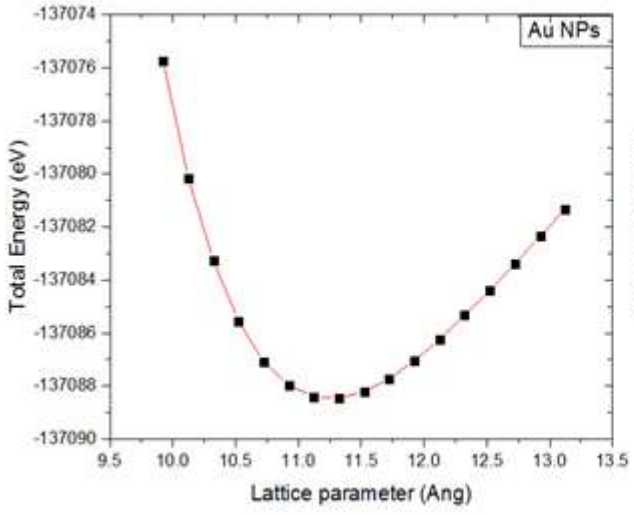
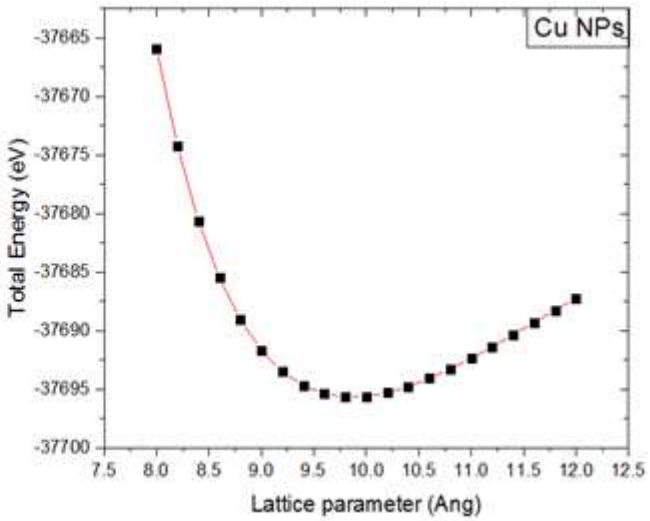


Figure 1: (a) Au NPs, (b) Cu NPs and (c) Au-Cu NPs with 13 atoms generated with ASE Program using the WUlff-constrction method

3. Results and discussion

We first present the results for structural properties. In order to obtain the equilibrium volume, we calculated the total energy for the Au NPs, Cu NPs and Gold-Copper NPs by varying hydrostatically the volume and allowing fully relaxation of the ions. The resultsare shown in Figure 2.The equilibrium lattice parameter was found using the GGA functional. The calculated results for equilibrium lattice are summarized in the Table 1.





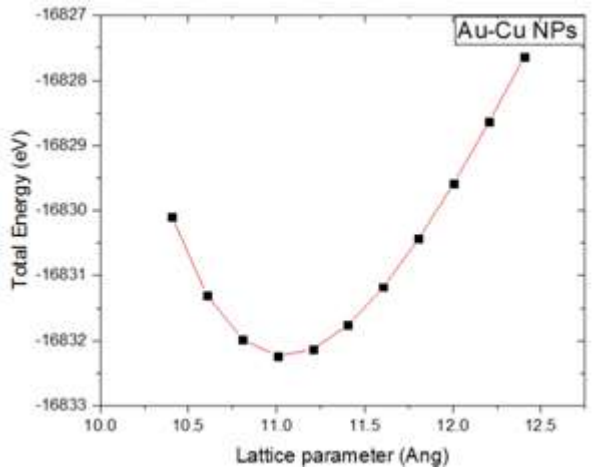


Figure 2: The calculated energy VS. Lattice parameter curves for optimizing the lattice constants as (a_{Au}, a_{Cu} and a_{Au-Cu})NPs.

Table 1: First principles structural and bulk modulus of Au, Cu and Au-Cu NPs

Materials	a_0(Ang)	K_0 (GPa)
Au NPs	11.32277	11.3
Cu NPS	9.80072	12.0
Au-Cu NPs	11.00800	13.5

We now turn the attention to the bulk modulus calculation. In order to obtain the equilibrium volume we calculated the pressurefor the Au, Cu and Au-Cu NPs. The resultsare shown in Figure 3.The bulk modulus K_0 was determined from the results of total energy change with respect to the hydrostatic variation of volume and fitted to the fourth-order Birch-Murnaghan equation of state. These resultsin bulk modulusas summarized in the Table 1.

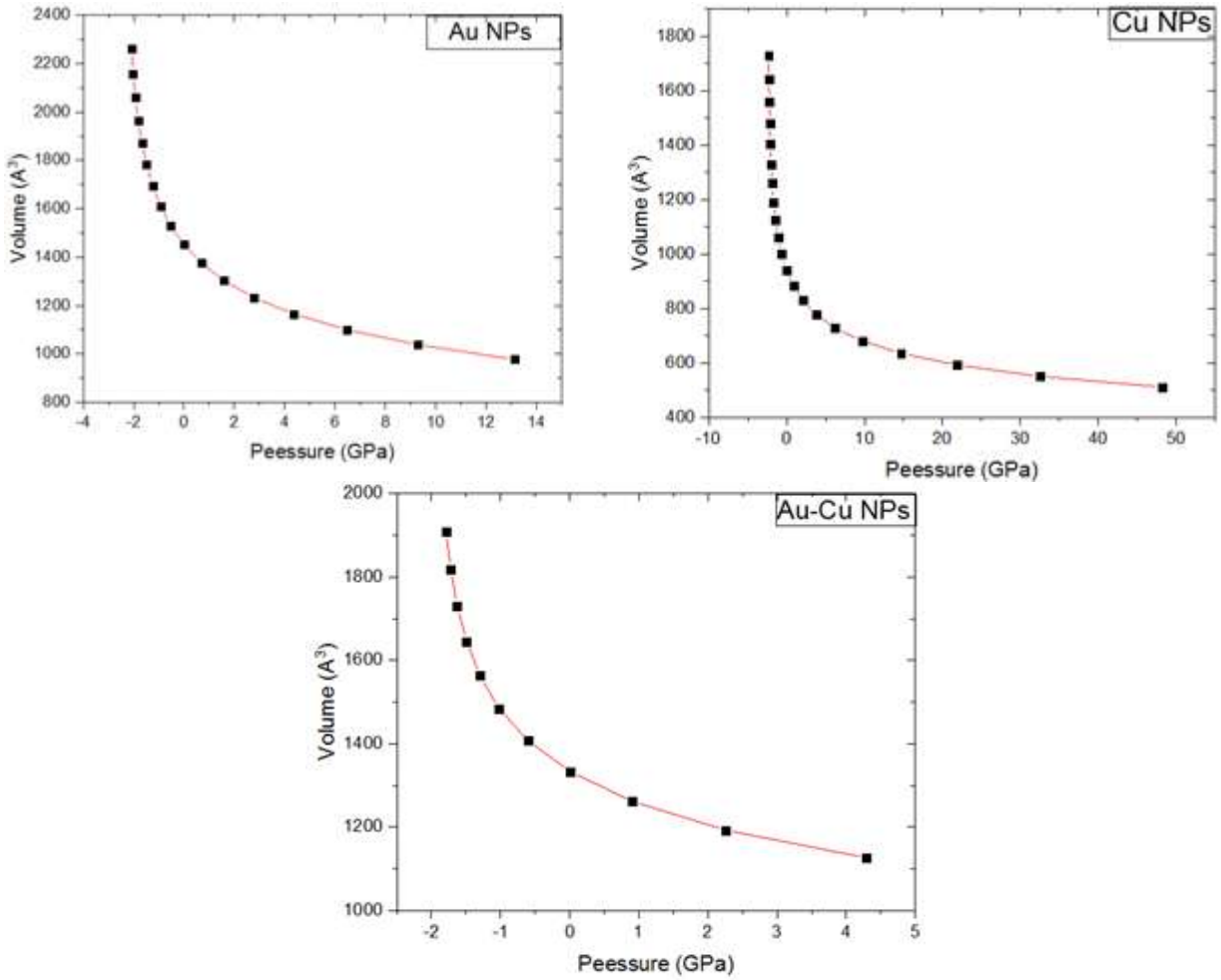


Figure 3: Compression data of (Au , Cu and Au-Cu) NPs at zero temperature. The solid curve is a least squares fit of the first-principles calculations data

4. Conclusion

In summary, we have presented first principles calculations of the lattice constant and bulk modulus of Au, Cu and Au-Cu NPs. Using DFT with Quantum Espresso package, one based on a definition in terms of the lattice parameter derivative of the total energy and another in terms of the volume derivative of the pressure often used in simulations. Both give quantitatively similar results.

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