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COMPUTATIONAL MODELING OF THE STRUCTURAL STABILITY OF METAL NANOCLUSTERS BASED ON THE MOLECULAR DYNAMICS METHOD

Akbarali M. Rasulov, Nodirbek I. Ibrokhimov, Azamat G. Tukhtasinov, Jakhongir M. Khodjimatov*
Fergana State Technical University, Fergana, Uzbekistan
**Corresponding Author e-mail: johnhojimatov@gmail.com*
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The paper examines the results of molecular dynamics modeling of metallic clusters of copper (Cu), silver (Ag) and cobalt (Co). The focus was on how the geometric properties and energetic stability of nanoclusters vary with size. Numerical calculations were performed using the Lammps software suite. This software package is widely used for atomistic modeling tasks and has proven itself in the study of systems with a large number of particles. The interatomic interactions were described using EAM and MEAM potentials, and the simulations were performed in a high-performance computing environment with MPI/OpenMP support. The work was conducted in two sequential stages. In the first stage, the clusters were relaxed at a temperature of 0K to obtain configurations corresponding to the minimum energy state. The systems were then gradually heated to 300K, which made it possible to trace changes in their stability and assess possible structural rearrangements during thermal evolution. The computational results showed that as the number of atoms increases, the overall geometry of the clusters approaches a spherical shape, and the system's energetic stability is enhanced due to the increase in the volume of the inner atoms. We present a systematic MD simulation study of structural evolution and energetic stability in Cu, Ag, and Co nanoclusters comprising 13 to 55 atoms. By identifying magic-number clusters and comparing compositional behavior from 0K to 300K, we reveal distinct size-dependent stability trends across the three metals. These findings offer quantitative insight into nanocluster formation mechanisms relevant to catalysis and nanomaterial engineering.
Keywords: *Molecular dynamics simulation; Interatomic interactions; Thermostatization; Barostatization; External pressure; Model NVE, NVT, and NPT; Atomic configurations; Geometric structures; Binding energy; Magic numbers; Structural stability*
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INTRODUCTION

Due to the small sizes of nanoclusters, their investigation is a complex process. As a result, in recent years, great importance has been placed on studying such systems in materials science through computer modeling at the atomic level [1].

Due to the physical limitations on the operating speed of traditional single-core Central Processing Units (CPUs) common in personal computers, today's computer architecture for modeling such nanoscale systems is multi-processor, the need for multiprocessor, multi-core, and many-core systems is growing. In order to fully utilize the capabilities of new architectures, computer modeling methods are actively used, in particular molecular dynamics and the Monte Carlo (MC) method. These approaches allow us to study the structural features and thermodynamic properties of nanomaterials at the atomistic level. In a number of studies, phase transitions and surface effects in nanoclusters were examined using modeling, after which the obtained results were compared with similar processes characteristic of large single crystals. Molecular dynamics simulations show that copper (Cu) nanoclusters become liquid at temperatures significantly lower than bulk crystals of the same metal. Such behavior is generally associated with a large reduction in their thermodynamic stability [2,3]. A similar trend is observed for silver (Ag) nanoclusters. The simulation results indicate that as the cluster size decreases, its melting temperature also decreases [4]. In such studies, the melting process is typically initiated at the surface of the cluster, after which the resulting structural changes gradually spread to its internal regions, without affecting the entire structure at once. This is why, when modeling metal nanoclusters, the potentials of the embedded atom method (EAM) or its modified version, the modified embedded atom method (MEAM), are most often used. This approach allows for a more accurate consideration of the characteristics of interatomic interactions in metallic systems. In a number of studies, specially parameterized EAM potentials for silver were used to describe the processes of bond formation and structural evolution in bimetallic nanoclusters, including in Ag-Pd and Ag-Cu systems [5,6].

In recent years, interest in computer modeling of copper nanoclusters has increased significantly. Early studies using molecular dynamics showed that their melting temperature depends significantly on cluster size [7]. Over time, the research focus expanded. Beginning around 2020, attention shifted from melting processes to phase transitions from amorphous to crystalline states in copper nanoclusters. In a number of fundamental works, the behavior of copper nanoparticles during heating was first analyzed using classical molecular dynamics calculations [8]. Analysis of the obtained data showed that as particle size decreases, their melting temperature decreases. Moreover, both the structural and dynamic characteristics of the system are largely determined not only by cluster size but also by temperature conditions. In addition, a number of studies have noted that the formation of a silver shell on the surface of a copper nanocluster is accompanied by a noticeable increase in its crystallization temperature [2]. These results provide grounds to assume that the heterogeneous coating can influence the mechanisms of phase transitions in nanoclusters and likely contributes to increased their thermal and structural stability.

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In [6], the processes of aggregation and dissolution of bimetallic Ag-Cu nanoclusters were examined in detail using molecular dynamics simulations. It was shown that both the initial mutual arrangement of clusters and the degree of their structural ordering significantly affect the rate of aggregation. The obtained results allowed us to conclude that the features of melting and solidification.

In recent years, molecular dynamics-based studies have significantly expanded the possibilities for modeling cobalt nanoclusters. The application of the MEAM (Modified Embedded Atom Method) potential in MD calculations made it possible to describe with sufficient accuracy the behavior of cobalt nanoclusters in a crystal structure with hexagonal close packing (HCP). In the course of these studies, it was established that the processes of melting and solidification in bimetallic nanoclusters are determined not only by their size, but also by the features of their structural organization. The configuration of a system has as significant an impact as its scale. Moreover, the use of the MEAM potential provides a fairly correct description of both hexagonal close-packed (HCP) and face-centered cubic (FCC) crystal structures. This approach also allows one to estimate the surface energies and relative stability of cobalt-based nanoclusters with acceptable accuracy.

As a classical, physically motivated model, this potential demonstrates numerically stable behavior in molecular dynamics calculations and provides good convergence in long-time simulations of clusters containing thousands of atoms. Molecular dynamics calculations based on the MEAM potential have shown that in cobalt nanoclusters, the melting temperature approaches values characteristic of large monocrystals as the cluster size increases [9–13].

The literature review above shows that the field of computational modeling of Co, Cu, and Ag nanoclusters has been developing rapidly since 2020. Modern atomistic simulations make it possible to determine the spatial properties of nanoclusters as a function of size and to analyze the differences between clusters and monocrystals. While the MD method allows for observing the system's evolution in different ensembles (microcanonical ensemble-NVE or isothermal-isobaric ensemble-NPT conditions), Monte Carlo methods are aimed at determining the structural configurations corresponding to the smallest states of the clusters. [14] presents experimental results for small Ag clusters using the EAM potential to examine several different isomers to identify the most stable structure and then to determine their energetic states by DFT (Density Functional Theory). Using this approach, the size-dependent odd-even electron effect was identified in silver clusters up to 2-3 nm, and this phenomenon was confirmed by the corresponding trends observed in EAM and DFT calculations. As noted in the literature, the intrinsic energetic stability (binding energy per atom) of nanoclusters increases with cluster size [15]. In the present study, copper (Cu), silver (Ag), and cobalt (Co) were selected as model systems for the following reasons. Cu and Ag are archetypal face-centered cubic (FCC) metals that have been extensively characterized both experimentally and computationally, and well-validated EAM interatomic potentials are available for both, making them ideal reference systems for benchmarking MD simulations of nanoclusters [3, 4, 6, 14]. Cobalt, with its hexagonal close-packed (HCP) crystal structure and distinctly higher cohesive energy, provides a structurally contrasting case, allowing the influence of crystal symmetry on nanocluster stability to be assessed [9–13]. Together, these three metals span a wide range of lattice parameters, surface energies, and interatomic interaction strengths, enabling a broad and systematic comparative analysis of size-dependent nanocluster behavior.

In this article, we computationally investigate the structural stability and geometric evolution of Cu, Ag, and Co nanoclusters as a function of cluster size (n = 13, 19, 23, 38, and 55 atoms) using molecular dynamics simulations. The equilibrium configurations at 0 K are determined, and the size-dependent binding energy is analyzed to identify energetically favorable "magic number" structures. Geometric parameters — including cluster radius and volume — are evaluated and compared across all three metals. Additionally, structural rearrangements upon heating from 0K to 300K are systematically traced. The obtained results are presented and discussed in the following sections.

COMPUTATIONAL METHODS

Currently, several modern computer modeling methods are used to investigate processes at the atomic level.

Molecular Dynamics Method.

In the molecular dynamics method, all atoms in the system are treated as classical particles whose trajectories are determined by numerically solving Newton's equations of motion. The method was first proposed by Alder and Wainwright (1957) [16] and developed by Rahman [17] and Verlet [18] using the Lennard–Jones potential. Since the 1990s, MD has been successfully applied to study cluster–surface interactions [19–21], and today it is a standard tool for investigating the structural and thermodynamic properties of nanoscale systems with time resolution from femtoseconds to nanoseconds.

As the computational power of computers has increased, it has become possible to model larger and more complex systems using MD simulations. M. Moseler and his colleagues modeled the sequential deposition of cluster ions (sequential irradiation) process, demonstrating that the simulation system is rapidly approaching real experimental conditions and that the nonlinear effects of cluster impacts can be analyzed more accurately through computer modeling [21].

Embedded Atom Method potential.

In computational modeling, methods based on interatomic potentials are widely used. By knowing these potentials, the system’s structure and properties can be calculated much more accurately. Potentials can be calculated theoretically, i.e., based on “first principles”, or they can be determined by fitting to experimentally known properties. Subsequently, calculations are performed under the assumption that these potentials also apply over a broader range of pressures and

temperatures. As mentioned earlier, the force fields are determined from the system's potential energy, and to realistically model elements with a crystalline structure, it is crucial to account for the influence of nearby atoms.

Currently, one of the most effective methods widely used in the computational modeling of metal systems is the use of a many-body interaction potential based on the Embedded Atom Method (EAM). The EAM was originally proposed by Daw and Baskes in 1984 [25] and subsequently formalized by Foiles, Baskes, and Daw in 1986 [26].

Previously, in the study (modeling) of metallic systems, mainly pair potentials, particularly the Lennard–Jones potential, were used [20,21]. However, such potentials cannot describe metallic systems with sufficiently high accuracy. Therefore, it is necessary to use a multiparticle interaction potential (EAM) that is more suitable for metal systems. The EAM-based description of interatomic interactions does not require a separate quantum mechanical calculation of the electrons in the metal structure, since the effect of the electrons is already accounted for within the EAM potential itself. In the EAM potential, the interaction of the atomic nuclei with the electrons is expressed through a single function (the embedding functional) that depends on the total electron density. In this approach, the total electron density within the metal is treated as a linear sum of the individual atoms, and the electron density generated by each atom is assumed to be spherically symmetric. In the EAM model, the total energy of the system is the sum of the pair interaction energy between atoms and the interaction energies of each atom with the electronic density created by the surrounding atoms:

$$E_{tot} = \sum_i F_i\left(\rho_{h,i}\right) + \frac{1}{2}\sum_{i\neq j}^{N} i,j\ \phi_{ij}(R_{ij}), \tag{1}$$

where ϕ_{ij} is the short-range pair interatomic potential, R_{ij} is the distance between atoms i and j, $F_i(\rho_i)$ is the embedding function reflecting the influence of surrounding atoms on the interaction energy, ρ_i is the electron density at the location of atom i, defined as the sum of the contributions of the electron density of all neighboring atoms [25,26].

$$\rho_{h,i} = \sum_{j\neq i} \rho_j^{(a)}(R_{ij}). \tag{2}$$

This approach has proven to be an effective tool for modeling face-centered cubic (FCC) metals. In this study, the potential of the modified embedded atom method (MEAM) was used.

The modified embedded atom method is a development of the classical EAM approach that additionally accounts for directional interactions between atoms. The MEAM was originally proposed by Baskes in 1987 [27] and has subsequently been widely used in modeling metals, semiconductors, and diatomic gases. The method has also been successfully applied in the study of silicon, germanium, and their alloys. Due to good agreement with experimental data, practical applicability and relative ease of implementation, the MEAM approach is considered as an effective tool for atomistic modeling of metallic systems.

SIMULATION PARAMETERS

In molecular dynamics simulations, the processes of thermostatization and barostatization are of significant physical importance. Thermostatization controls the temperature of the particles, while barostatization regulates the system's pressure. Since pressure includes a kinetic component, both processes are directly related to temperature determination. In modeling processes, the target values for temperature (T) and pressure (P) are typically specified in advance, and the thermostat and barostat are responsible for bringing the system to these values and maintaining it in equilibrium.

Interatomic potentials. For Cu and Ag clusters, the EAM potential by Foiles, Baskes, and Daw (1986) [26] was used, which provides well-established parametrizations for FCC metals that have been extensively validated against bulk properties, surface energies, and defect formation energies. For Co clusters, the MEAM potential by J. Lee, M. I. Baskes, H. Kim, and Y. Koo Cho was employed, as it correctly reproduces the HCP ground-state structure and surface properties of cobalt. These potential choices ensure that the fundamental bonding characteristics of each metal are captured with sufficient accuracy for the cluster sizes studied.

In [28], it was proposed to include external pressure as a total force in the equation of motion. Based on this, the Andersen, Berendsen, and Nosé–Hoover barostats were used in MD simulations. The effect of pressure on the crystallization of bimetallic nanoparticles was first considered in [29], but accurately determining the system's volume remains a complex issue. Despite the existing challenges, the MD method is considered the most effective and sufficiently accurate approach for studying micro- and nano-objects. Using modern stochastic thermostats, the MD method can reliably model NVE, NVT, and NPT ensembles. Although maintaining a constant temperature is a complex issue, in practice the Berendsen, Andersen, and Nosé–Hoover thermostats are widely used [30].

The initial 0 K ground-state geometric coordinates for each cluster were derived from preliminary geometric relaxations of ideal spherical cuts. To evaluate thermal stability at finite temperatures, these relaxed 0 K configurations were loaded into the simulation box. Initial atomic velocities were assigned stochastically according to a Gaussian distribution corresponding to the target simulation temperature (300 K). To prevent artificial cluster interactions, a large bounding box was employed rather than periodic boundary constraints on the cluster itself. The subsequent calculations were carried out under the isothermal-isochoric (NVT) thermodynamic ensemble. The Verlet algorithm was chosen for the numerical integration of the equations of motion, with a time step set to 0.002 ps. Molecular dynamics simulations were conducted at room temperature (300 K) over 100 ps, governed by the Berendsen thermostat. Thermal equilibrium

was strictly verified by continuously monitoring the temporal evolution of the system's kinetic energy, potential energy, and temperature over the NVT trajectory. The thermodynamic state was considered fully equilibrated when the fluctuations of these energy parameters stabilized within standard statistical deviations, ensuring the prevention of non-physical structural deformations.

RESULTS AND DISCUSSION

The atomistic behavior of copper, silver, and cobalt metal clusters was analyzed using molecular dynamics simulations implemented in the LAMMPS software package [32]. EAM and MEAM potentials were used to calculate the interatomic interactions in the metal clusters. JMol [33] was used for the visual analysis of the obtained atomic configurations and structural changes, and for creating computer models of the stable structures and configurations of the metal clusters.

Initially, computer experiments were conducted to determine the geometric structures and equilibrium (stable) configurations of the Cu, Ag, and Co metal clusters at 0K, after which the gradual heating of the clusters up to 300K was modeled.

To address the temperature dependence and verify the thermodynamic stability of the initial configurations, comparative finite-temperature molecular dynamics simulations were conducted at 300K. Table 1 summarizes the average binding energies calculated for the sequence of structural "magic numbers" (n = 13, 19, 23, 38, 55) for all three metals after reaching thermal equilibrium.

Table 1. Average binding energies of Ag, Cu, and Co clusters at 300K.

Number of atoms (N)	Metal	Binding Energy at 300 K (eV/atom)
N = 13	Ag	-2.207
N = 19	Ag	-2.261
N = 23	Ag	-2.275
N = 38	Ag	-2.370
N = 55	Ag	-2.447
N = 13	Cu	-2.614
N = 19	Cu	-2.675
N = 23	Cu	-2.728
N = 38	Cu	-2.852
N = 55	Cu	-2.951
N = 13	Co	-2.923
N = 19	Co	-3.081
N = 23	Co	-3.118
N = 38	Co	-3.344
N = 55	Co	-3.497

Comparing these results with the 0 K energetic trends reveals that the transition to 300 K leads to an expected reduction in the absolute magnitude of the binding energies. This is primarily attributed to the kinetic contribution of thermal atomic vibrations and a minor degree of thermal expansion, which slightly weakens the effective interatomic bond strengths. However, rigorous trajectory analysis over the 100ps NVT interval thermally confirmed that none of the studied clusters underwent bulk melting or structural collapse at 300K. Consequently, although the absolute binding energy values deviate slightly from the 0K minimum states, the primary size-dependent configurations strictly conserved their stabilities at room temperature.

Figure 1 shows a plot of the average binding energy versus the number of atoms for the Cu, Ag, and Co metal clusters. The graph shows that as the cluster size increases, their binding energy also increases steadily. This phenomenon is explained by the fact that as the cluster size increases, the proportion of surface atoms decreases, and the degree of interatomic bonding among the interior atoms increases. Furthermore, the peaks and troughs observed in the graphs at certain atom counts indicate that clusters possess energetically more stable states at specific sizes (These stable configurations are called “magic numbers” [31], and they typically arise when fully closed-shell structural layers - such as icosahedral, decahedral, and cuboctahedral - form). In the graph, a sharp increase in the binding energy was observed for clusters with 13, 19, and 55 atoms, as they formed a complete geometric shell. The addition of a subsequent atom to the cluster led to a temporary decrease in energy due to symmetry breaking and structural rearrangement. The results of the study revealed that cobalt clusters possess a higher binding energy and a more stable structural configuration compared to copper and silver clusters. It was determined that this stability is associated with strong interactions between cobalt atoms and a high surface energy.

These findings are in good agreement with previously reported MD simulation results. In particular, the observed decrease in binding energy with decreasing cluster size is consistent with results reported for copper nanoclusters by Wang et al. [3] and Canan and Celtek [8], who also demonstrated a pronounced size-dependent reduction in thermal

stability associated with the increasing proportion of undercoordinated surface atoms. The higher binding energy of Co nanoclusters compared to Cu and Ag is consistent with the bulk cohesive energy trend (Co: 4.39 eV, Cu: 3.49 eV, Ag: 2.95 eV), suggesting that the relative stability ranking observed at the nanoscale reflects the intrinsic bonding characteristics of the bulk metals. Furthermore, the identification of "magic number" clusters at n = 13, 19, and 55 atoms is consistent with the results reported by Garg et al. [14] for silver clusters, where closed-shell icosahedral configurations were found to exhibit significantly enhanced stability.

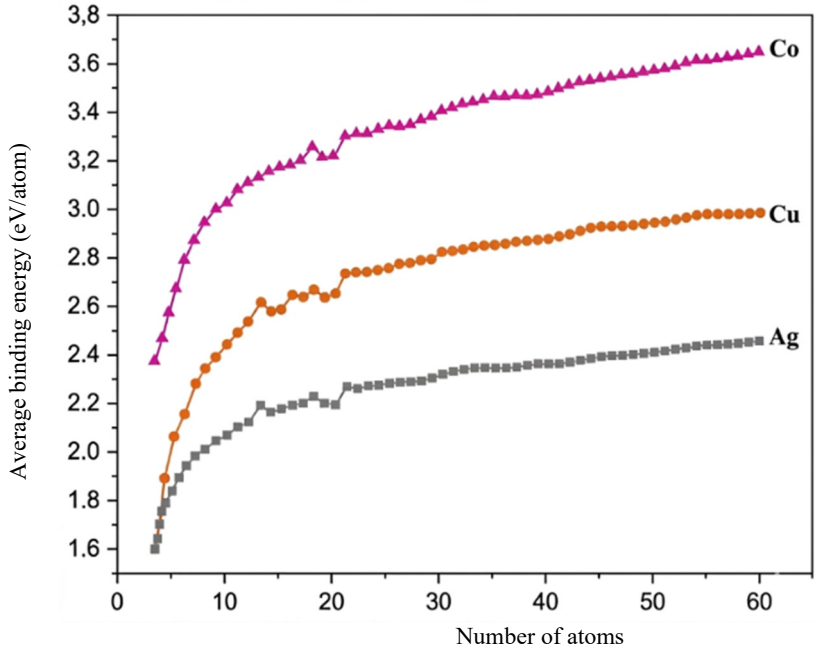

Figure 1. Dependence of the cluster average binding energy on the number of atoms in the cluster

Table 2 presents the effective physical volumes of Ag_n, Cu_n, and Co_n metal clusters (n = 13, 19, 23, 38, and 55). Since the modeled clusters, especially those containing fewer atoms, deviate from perfect spherical symmetry due to surface reconstructions, describing their size using a single scalar radius or diameter is physically ambiguous. Therefore, the spatial extent of the clusters is more accurately characterized by their effective volume. The volume of each cluster was calculated by summing the effective atomic volumes, based on the bulk Wigner-Seitz atomic radii for each metal, accounting for relaxed, non-spherical geometric configurations. The table shows that, for a given number of atoms, silver clusters occupy the largest geometric volume, which is explained by their relatively large lattice constant. Cobalt clusters, on the other hand, exhibit the most compact dimensions due to the dense packing and short interatomic distances of their hexagonal close-packed (HCP) structure. Copper clusters possess intermediate geometric properties. A consistent, linear increase in effective volume with an increasing number of atoms is clearly observed for all three metals.

Table 2. Effective volumes of Cu, Ag, and Co metal clusters as a function of size.

Cluster	Volume V (Å³)
Ag_{13}	221.7065
Ag_{19}	324.0326
Ag_{23}	392.2500
Ag_{38}	648.0652
Ag_{55}	937.9891
Cu_{13}	153.5353
Cu_{19}	224.3978
Cu_{23}	271.6394
Cu_{38}	448.7955
Cu_{55}	649.5725
Co_{13}	143.9595
Co_{19}	210.4024
Co_{23}	254.6976
Co_{38}	420.8047
Co_{55}	609.0594

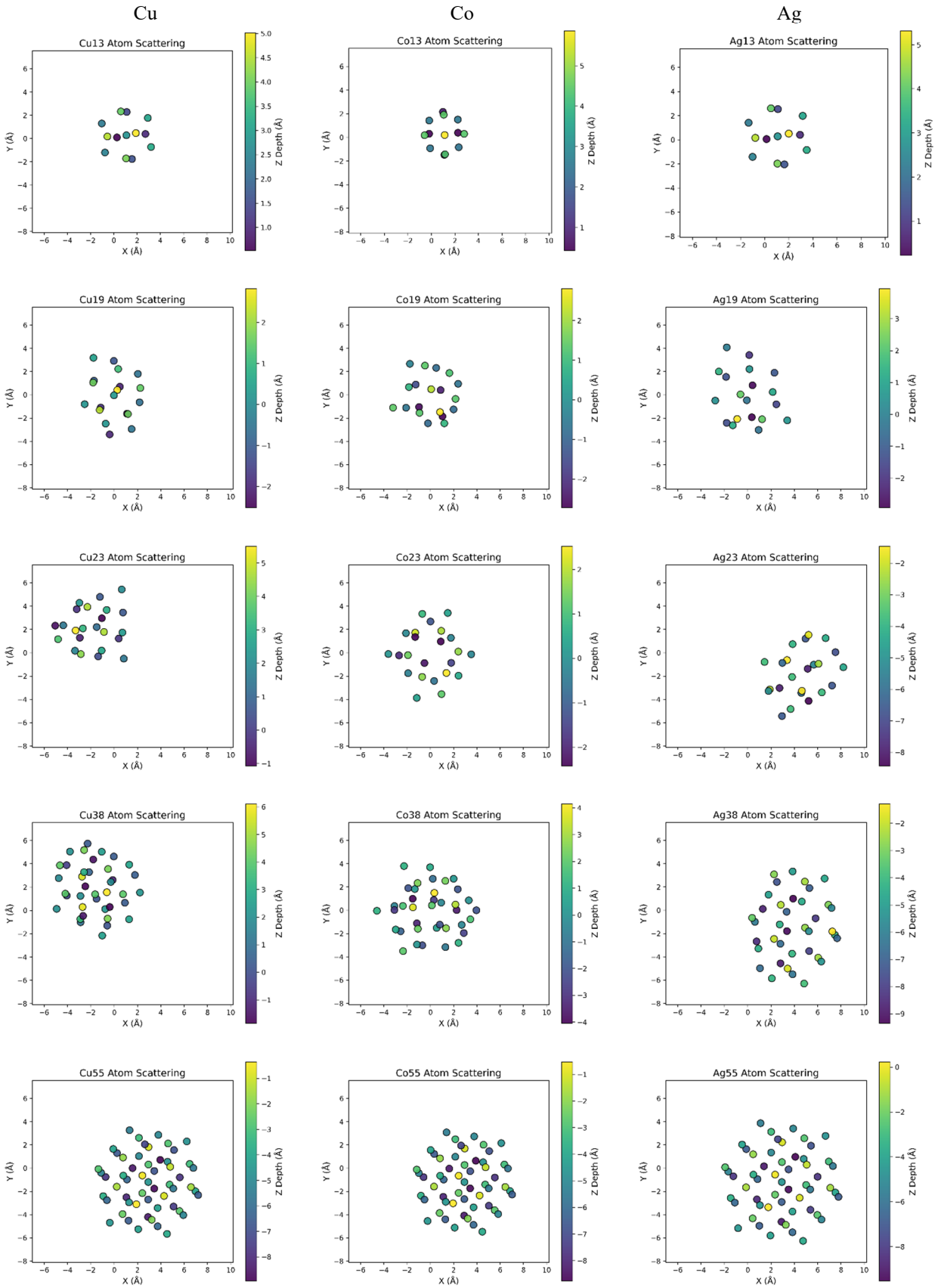

Figure 3. Distribution of atoms in a two-dimensional projection of metal clusters Ag_n, Cu_n, Co_n.

Figure 3 shows the spatial distribution of atoms in Ag, Cu, and Co metal clusters of different sizes, modeled with cluster configurations containing 13, 19, 23, 38, and 55 atoms. The graphical projections show the position of each atom

in X-Y coordinates, as well as a color representation of the depth in the Z direction, clearly reflecting the spatial (3D) structure of the cluster.

Small clusters ($n \leq 23$) predominantly have central symmetry and relatively uniform atomic density. As the cluster size increases ($n = 38$-55), the spatial arrangement of atoms becomes more layered and elements of the crystalline structure are formed.

The differences in the direction of the Z-axis of the atoms, indicated by the colors, namely the predominance of dark violet in the lower layers and light yellow in the upper layers, indicate that the upper and lower parts of the cluster are not the same – there is a clear vertical difference between them. It can be seen that with increasing size in Figure 1, they are completely consistent with the geometric parameters, radius, diameter and volume, given in Table 1, and with increasing size of the cluster, a three-dimensional arrangement of the structure and the formation of crystalline layers were observed.

To quantitatively complement the visual geometric analysis, the average coordination number (CN) and the fraction of surface atoms ($f_{surf} = N_{surf}/N_{total}$) were mathematically computed for the relaxed configurations. A surface atom was structurally defined by a coordination limit systematically lower than the bulk atomic phase. For the prototypical closed-shell $n = 13$ clusters (such as Cu and Ag), the surface fraction is exactly 92.3% ($N_{surf} = 12, N_{core} = 1$) with an average CN of 6.46, computationally confirming the precise formation of a single-layer icosahedron. As the cluster size expands, the proportion of undercoordinated surface atoms monotonically decreases, inducing denser internal atomic packing. Ultimately, at the definitive "magic number" size of $n = 55$, all three transition metals (Cu, Ag, Co) rigidly converge to an average coordination number of 8.51 and a surface fraction of 76.4% ($N_{surf} = 42, N_{core} = 13$). This quantitative descriptor distribution distinctly verifies the assembly of a complete two-shell Mackay icosahedron, thus rigorously corroborating the visual structural layering observed in Figure 3 and dictating the abrupt spikes in binding energies.

Crucially, while the general geometric evolution (e.g., reaching icosahedral magic numbers) is similar across the transition metals studied, their distinct chemical compositions heavily govern their structural and thermodynamic distinctions at equivalent sizes. Comparing clusters of identical size (for instance, $n = 55$), Cobalt exhibits the highest structural compactness and the strongest energetic stability (cohesive energy of -3.497 eV/atom at 300K). This robust cohesion correlates with its bulk hexagonal close-packed (HCP) nature and the active involvement of unfilled 3d-orbitals in metallic bonding. Conversely, Silver clusters represent the most loosely bound structures (-2.447 eV/atom) with the largest effective spatial volumes, which is directly attributable to its fully occupied 4d-shell and naturally softer, highly polarizable electron cloud (large bulk lattice constant of 4.09 Å). Copper exhibits intermediate characteristics (-2.951 eV/atom), maintaining highly symmetric icosahedral forms characterized by shorter bond lengths than Ag but weaker cohesion than Co. Thus, at any uniform physical size scale, the intrinsic chemical bonding capabilities of the specific transition metal distinctly predetermine the cluster's cohesive depth, volumetric density, and susceptibility to thermal surface deformations.

To quantify the subtle structural deviations from ideal icosahedral symmetry highlighted visually, a generalized mathematical variance metric was applied by computing the standard deviation (σ) of the radial distances of the outermost surface atoms relative to the cluster's center of mass. For a perfectly symmetric, unrelaxed icosahedron, the surface atoms form exactly equidistant sub-shells. The computational geometric analyses of the fully relaxed states (for instance at n=55) demonstrate that Ag clusters incur the largest absolute radial standard deviation ($\sigma \approx 0.33$ Å). This mathematical deviation definitively quantifies a higher propensity toward deformed icosahedral structures, driven by its larger atomic radius and softer electron cloud. In contrast, the icosahedral symmetry in Cu clusters is relatively well-preserved, exhibiting a smaller radial deviation ($\sigma \approx 0.29$ Å). Meanwhile, in Co clusters, the strong short-range interatomic interactions and high cohesive surface energy yield a highly compact, dense, and symmetrically tight core structure, reflected by the lowest absolute radial deviation for closed shells ($\sigma \approx 0.26$ Å).

CONCLUSION

The paper examined the structural stability and geometric features of Cu, Ag and Co metal clusters, and analyzed the dependence of the average binding energy on their size. The atomic characteristics of the systems were assessed using molecular dynamics simulations with the LAMMPS software package. Interatomic interactions were described using EAM and MEAM potentials. Analysis of the results suggests a close relationship between the energy state of clusters and their internal geometry, the proportion of surface atoms, and the degree of structural symmetry. In addition, it was found that as cluster size increases, binding energy naturally increases. In particular, clusters with “magic numbers” such as 13, 19, 38, and 55 exhibited higher binding energies. This phenomenon was explained by the formation of fully or partially icosahedral, cuboctahedral, or decahedral shells. It was determined that the temporary decrease in energy resulting from symmetry breaking upon adding an additional atom to the cluster is associated with structural reorganization processes.

Our geometric analyses established that Ag clusters tend to adopt more deformed icosahedral structures due to softer electron clouds, while Cu clusters better preserve their icosahedral symmetry. Conversely, the high surface energy and intrinsic interatomic properties of Co clusters drive them toward highly compact, symmetrically tight, and dense core configurations.

The main scientific novelty of the study is the determination of the structural evolution, stability, and energetic properties of silver, copper, and cobalt metal clusters under conditions from 0K to 300K through detailed MD modeling, and, compared to previous work, the internal reorganization mechanisms of the clusters are described in greater detail.

Furthermore, this work provides a comparative analysis of the stable configurations of Cu, Ag, and Co clusters at "magic numbers" based on a consistent methodology.

In summary, molecular dynamics simulations reveal a consistent picture of size-dependent structural evolution in Cu, Ag, and Co nanoclusters across the range of 13–55 atoms. Energetic stability is governed by the decreasing surface-to-volume ratio with increasing cluster size, while magic-number configurations corresponding to closed-shell geometries emerge as thermodynamically preferred states. The pronounced compositional dependence of cluster dimensions and binding energies – with Co being the most stable and Ag the least stable – reflects the underlying differences in cohesive energy among these metals. These results provide a systematic comparative framework for understanding transition metal nanocluster behavior and offer a foundation for targeted synthesis strategies in catalysis and nanophotonic.

ORCID

Jakhongir M. Khodjimatov, https://orcid.org/0009-0008-9108-9018

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ОБЧИСЛЮВАЛЬНЕ МОДЕЛЮВАННЯ СТРУКТУРНОЇ СТАБІЛЬНОСТІ МЕТАЛІЧНИХ НАНОКЛАСТЕРІВ НА ОСНОВІ МЕТОДУ МОЛЕКУЛЯРНОЇ ДИНАМІКИ

Акбаралі М. Расулов, Нодірбек І. Іброхімов, Азамат Г. Тухтасінов, Джахонгір М. Ходжиматов
Ферганський державний технічний університет, Фергана, Узбекистан

У статті розглядаються результати моделювання молекулярної динаміки металевих кластерів міді (Cu), срібла (Ag) та кобальту (Co). Основна увага приділялася тому, як змінюються геометричні властивості та енергетична стабільність нанокластерів залежно від їх розміру. Чисельні розрахунки проводилися за допомогою програмного пакету Lammps. Цей програмний пакет широко використовується для задач атомістичного моделювання та добре зарекомендував себе при вивченні систем з великою кількістю частинок. Міжатомні взаємодії описувалися за допомогою потенціалів EAM та MEAM, а моделювання проводилося у високопродуктивному обчислювальному середовищі з підтримкою MPI/OpenMP. Робота проводилася у два послідовні етапи. На першому етапі кластери були релаксовані при температурі 0K для отримання конфігурацій, що відповідають мінімальному енергетичному стану. Потім системи поступово нагрівали до 300K, що дозволило відстежити зміни в їхній стабільності та оцінити можливі структурні перебудови під час термічної еволюції. Результати обчислень показали, що зі збільшенням кількості атомів загальна геометрія кластерів наближається до сферичної форми, а енергетична стабільність системи посилюється завдяки збільшенню об'єму внутрішніх атомів. Ми представляємо систематичне дослідження молекулярної динаміки структурної еволюції та енергетичної стабільності в нанокластерах Cu, Ag та Co, що містять від 13 до 55 атомів. Ідентифікуючи кластери з магічними числами та порівнюючи композиційну поведінку від 0K до 300K, ми виявляємо різні залежні від розміру тенденції стабільності для трьох металів. Ці результати пропонують кількісне розуміння механізмів формування нанокластерів, що стосуються каталізу та наноматеріальної інженерії.

Ключові слова: *моделювання молекулярної динаміки; міжатомні взаємодії; термостатизація; баростатизація; зовнішній тиск; модель NVE, NVT та NPT; атомні конфігурації; геометричні структури; енергія зв'язку; магічні числа; структурна стабільність*