Semiconductor Optoelectronics
ISSN: 1001-5868

REGULARITY OF FORMATION OF MONO-I BIMETALLIC NANOPARTICLES IN THE COALESCENCE PROCESS

Ali Nasir Abdul Hussein
Ministry of Education, Iraq

Abstract

We performed simulations to study the fusion process of metal nanoparticles made of nickel, aluminum, copper, silver and gold. We used two different methods: the Monte Carlo method and the molecular dynamics method. The nanoparticles were subjected to gradual thermal exposure during the simulations, and mono- and bi-metallic systems were taken into account. The nanoparticles were designed as spheres and two perpendicular blocks. Our study revealed significant differences in the evolution of the fusion process between mono- and bi-metallic nanoparticles. We observed that several properties varied significantly, including the coalescence temperature, the structure and shape of the neck formed between the nanoparticles, and the dihedral angle between them. But it is possible to accurately predict the behavior of a bimetallic system during the fusion process based on the fusion behavior observed in a monometallic system containing the same constituent metals. This indicates the complexity of the fusion process in bimetallic systems, and highlights the need for further research in this area. Overall, the study provides valuable insights into the coalescence behavior of metal nanoparticles and emphasizes the importance of considering the specific properties of bimetallic systems.

Keywords: mono- and bimetallic nanoparticles, molecular dynamics, coalescence, Monte Carlo method, molecular dynamics method, dihedral angle.

Introduction:

The study of nanoparticles has opened up new avenues in nanotechnology that were previously inaccessible. Nanoscale particles possess tunable properties that can lead to the development of novel materials with unique structures. The wavelength of light emitted by quantum dots is one of the properties that depends on the size of the nanoparticle. The full spectrum of visible light can be generated with precise adjustment of their diameter. In addition, each nanoparticle has an internal atomic structure that is randomly oriented relative to other nanoparticles, which in turn contributes to the distinct physical properties of nanoparticle assemblies. Given their wide applications, from optical coatings and corrosion-resistant coatings to photocatalysts and solar energy devices, and from intravitreal implantable devices and surgical coatings to chemical reactors and semiconductor components, industrial interest in nanoparticle technologies is expected to continue in the coming years [1].

In practical applications, particularly in functional materials characterized by a high surface area, precise control over the porosity and resulting structure of thin films derived from nanoparticles is of utmost importance. These factors play a crucial role in determining numerous other physical properties. For instance, in sensor applications, efficient electronic conduction is facilitated, and the resulting electrical signal is significantly enhanced through the formation of junctions among

nanoparticles, thereby minimizing contact resistance. Throughout the process of film growth, particles interact with one another, leading to the aggregation of primary particles into nanoclusters or the partial/complete merging of nanoclusters and small nanoparticles, resulting in the formation of larger nanoparticles or nanoparticle aggregates. The formation of thin films then takes place through sintering mechanisms. As a result, it is not surprising that extensive experimental and theoretical research has focused on comprehensively understanding and modeling these mechanisms. Regardless of the simplicity or complexity of these models, they yield consistent outcomes. The driving mechanism behind sintering is the minimization of the free energy of the system, achieved by decreasing the interfacial energy, mainly through atomic surface diffusion. This process results in the development of a neck region with variable width between nanoparticles, leading to a reduction in the curvature radii of the nanoparticle pairs. Under specific conditions such as temperature, particle size, and composition, complete coalescence of nanoparticles can take place.

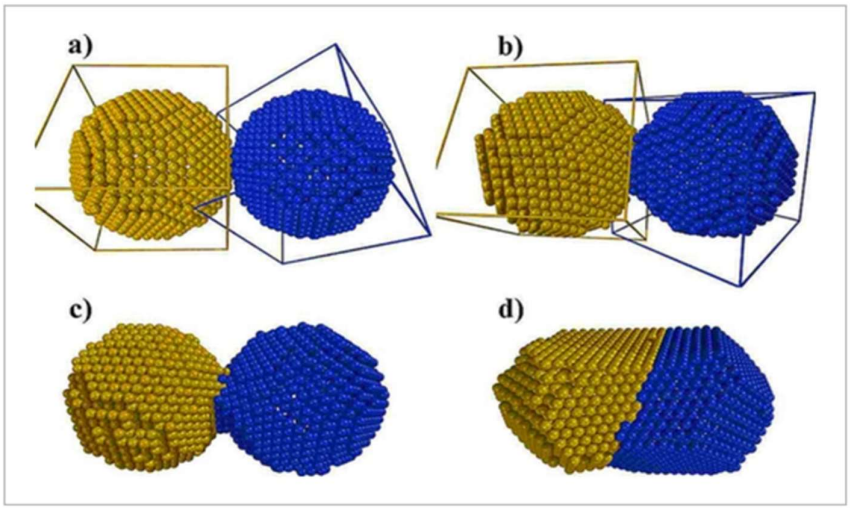


Figure 1. Stages of merger formation

Thus, investigating the factors and conditions governing the formation of mono- and bimetallic nanoparticles is crucial for both fundamental and applied science. Computer modeling of such systems allows for predicting optimal conditions for the functioning of nano-devices based on them and revealing specific behavioral characteristics when experimental studies are labor-intensive and financially costly [4-5].

From a nanomaterial perspective, the stages leading to the formation of twin boundaries during the merging process can be described as follows:

1. Close proximity of the clusters: At this stage, the two clusters of nanoparticles approach each other closely due to various factors such as diffusion, external forces, or thermal effects.

2. Interaction and alignment: The clusters interact and experience attractive forces, causing them to align their crystallographic orientations. It is important for the nanoparticles to have compatible lattice structures for favorable alignment [6]

3. Atomic diffusion and rearrangement: As the clusters continue to approach each other, atomic diffusion takes place. Atoms migrate across the interface, rearranging themselves to achieve a more energetically favored configuration. This diffusion can be facilitated by processes like

vacancies, interstitials, or grain boundary diffusion.

4. Twin boundary formation: The final stage involves the completion of the merging process, resulting in the formation of a twin boundary. A twin boundary is a special type of interface characterized by a mirror-like symmetry across which the crystal lattice is twinned. It arises from the rearrangement of atoms and differences in crystal orientations between the merged clusters [7]

Overall, the stages from cluster proximity to the formation of a twin boundary involve a sequence of interactions, alignment, atomic rearrangement, and finally the establishment of a distinct boundary. These processes contribute to the unique properties and characteristics of nanomaterials exhibiting twin boundaries.

Problem Statement:

The objective of this study was to conduct computer simulations using the Monte Carlo (MC) and molecular dynamics (MD) methods to investigate the coalescence process of mono- and bimetallic nanoparticles with predefined shape and structure. The results obtained from the MC method were compared with the molecular dynamics (MD) method, and then the conditions for the formation of necks between mono- and bimetallic nanoparticles were analysed. The Gupta many-body potential [6], with parameters taken from a previous study [7], was used to describe the atomic interactions. All calculations were performed using software developed within our research group: the NanoExpert program [8] was used for the MC method, and the ClusterEvolution program [9] was utilized for the MD method. The study aimed to explore the coalescence behavior of nanoparticles and understand the factors influencing the formation of neck structures. By employing computer simulations, the researchers aimed to gain insight into the underlying mechanisms and provide valuable information for the design and optimization of nanoparticle-based devices and materials. Overall, the task at hand involved simulating the coalescence process of mono- and bimetallic nanoparticles using the MC and MD methods, comparing the results, and analyzing the conditions for neck formation using the Gupta potential.

Methodology:

1. **Selection of Nanoparticles and Materials:**

The selection of metal nanoparticles for this study was based on their relevance to various applications and the distinct properties exhibited by each metal. The metals chosen included nickel, aluminum, copper, silver, and gold. These metals are widely used in different fields due to their unique characteristics. Nickel nanoparticles are known for their excellent mechanical and magnetic properties, making them suitable for applications in catalysis, magnetic storage devices, and sensors [7]. Aluminum nanoparticles possess high thermal conductivity, corrosion resistance, and lightweight properties, making them beneficial in industries such as aerospace and automotive. Copper nanoparticles exhibit excellent electrical conductivity and are commonly used in electronics, conductive inks, and catalysts. Silver nanoparticles are well-known for their antimicrobial properties, optical properties, and high electrical conductivity. They find applications in various fields such as antibacterial coatings, optical devices, and conductive inks. Gold nanoparticles possess outstanding optical properties, stability, and biocompatibility, making them widely used in biosensing, drug delivery, and plasmonic applications [8]. By considering mono- and bimetallic systems, the study aims to investigate the behavior and interactions of these nanoparticles when they are combined. Bimetallic systems can exhibit synergistic effects, unique catalytic properties, and tailored functionalities compared

to individual metals. Therefore, studying the fusion process and coalescence behavior in both mono- and bimetallic systems provides valuable insights for understanding the behavior and potential applications of these nanoparticles in real-world scenarios. The selection of these metals and the investigation of both mono- and bimetallic systems ensure a comprehensive understanding of the coalescence process and the factors influencing it. This knowledge contributes to the development of advanced materials and enables the design and optimization of nanoparticle-based devices with enhanced properties and performance [10]

2. Simulation Methods:

Two simulation methods, Monte Carlo (MC) and molecular dynamics (MD), were used in this study to study the nanoparticle fusion process. The Monte Carlo method is a computational technique that uses random sampling to simulate the behavior of a system. In the context of this study, it was used to simulate the nanoparticle coalescence process. We used NanoExpert software specifically designed to simulate the behavior of nanoparticles. This software allowed them to model and analyze the interactions between selected metal nanoparticles during the fusion process. By running multiple iterations of the simulation with different parameters, we were able to obtain statistical data and insights into the progress and outcomes of the fusion process. On the other hand, molecular dynamics is a simulation method that models the movement and interactions of individual atoms or molecules over time. In this study, molecular dynamics simulations were applied to study the coalescence behavior of nanoparticles. ClusterEvolution software was used for this purpose [11]. This program allowed us to simulate the dynamics of nanoparticles, taking into account their atomic structure and the interatomic forces acting on them. By performing molecular dynamics simulations, we were able to monitor the path of nanoparticles during the fusion process, study the interactions between molecules, and analyze the resulting structural changes. By using Monte Carlo and molecular dynamics methods, the study aims to provide a comprehensive understanding of the coalescence behavior of selected metal nanoparticles. These simulation techniques have allowed the process to be investigated at different levels of detail, from statistical behavior to atomic dynamics. Combining these approaches has provided valuable insights into the mechanisms and factors affecting the fusion process, helping to elucidate the underlying physics and guide the design and optimization of nanoparticle systems for various applications[12].

3. Predefined Shape and Structure of Nanoparticles:

In this study, nanoparticles were deliberately designed with specific shapes and structures to explore their effect on the coalescence process. Two main geometries were chosen: spheres and two orthogonal blocks. Spherical nanoparticles are a popular choice in nanoscience research due to their simplicity and symmetry. Domains provide a uniform and regular format that allows results to be more easily analyzed and compared. By simulating the fusion of spherical nanoparticles, we aimed to understand the fundamental behavior and dynamics of particle fusion in a simplified scenario. In addition to the spheres, the study also incorporated nanoparticles with a more complex geometry, namely two orthogonal blocks. This design choice is intended to capture the effect of nanoparticle structure on the fusion process. By introducing this geometric arrangement, we sought to investigate how the specific shape and orientation of nanoparticles influence their coalescence behavior. The orthogonal blocks presented an asymmetric, non-spherical structure, providing a more realistic representation of some nanoparticles found in

experimental systems[13].To implement this aspect of the study, we implemented the selected designs using appropriate software tools and algorithms. They used 3D modeling software to create the desired spherical nanoparticles and mass based on pre-defined dimensions and parameters. However, we used mathematical algorithms and computational methods to computationally construct the nanoparticles, ensuring an accurate representation of their shapes and structures. By implementing and simulating these pre-defined shapes and structures, we were able to investigate the effect of geometric arrangements on the docking process. We were able to observe how different shapes and structures affect fusion behavior, including factors such as contact area, diffusion rates, and atomic rearrangements. This analysis contributed to a better understanding of the relationship between nanoparticle geometry and fusion dynamics, enabling us to make informed decisions and make progress in designing, synthesizing, and engineering nanoparticles for various applications[14]

4. Thermal Exposure and Gradual Temperature Increase:

We conducted a series of experiments in which nanoparticles were subjected to gradual thermal exposure. This approach allowed us to monitor and analyze the evolution of the fusion process with increasing temperature. The purpose of this gradual temperature increase was to study the temperature-dependent properties and behavior of nanoparticles during fusion. By systematically increasing the temperature, we were able to monitor and understand how the nanoparticle incorporation process changes in response to different thermal conditions. Through this thermal exposure, we can study various aspects, such as the effect of temperature on the diffusion rates of atoms within nanoparticles, changes in the contact area between nanoparticles as a result of temperature-induced restructuring, and the formation and stability of atomic atoms. Bonds during the fusion process. To achieve this, we carefully controlled the temperature in the simulations, gradually increasing it over a predetermined range. We recorded and analyzed changes in nanoparticle structure, morphology, and other relevant properties at each temperature step, allowing us to establish a comprehensive understanding of the temperature-dependent phenomena that occur during the fusion process[13-14] These experiments provided valuable insights into the role of temperature in nanoparticle fusion, highlighting the mechanisms and kinetics involved in nanoparticle fusion under different thermal conditions. The knowledge gained from this work can inform the design and improvement of nanoparticle fabrication methods, as well as enhance our understanding of temperature-dependent processes in nanomaterials. Overall, by implementing stepwise thermal exposure and observing the fusion process at increasing temperatures, we gained valuable insights into the temperature-dependent behavior of nanoparticles during fusion .for example Metallic Nanomaterial: Gold Nanoparticles (AuNPs) [15]

1. Effect of temperature on diffusion rates of atoms within nanoparticles: $Au(0) \rightarrow Au(1-\delta)$, where Au(0) represents gold atoms in nanoparticles at lower temperatures, and Au(1-δ) represents gold atoms with a slight decrease in the number of vacancies (δ) due to increased temperature.

2. Changes in contact area between nanoparticles as a result of temperature-induced restructuring: $AuNP^1 + AuNP^2 \rightarrow AuNP^3$, where $AuNP_1$ and $AuNP_2$ represent individual gold nanoparticles at lower temperatures, and $AuNP_3$ represents the fused or partially fused gold nanoparticle formed at higher temperatures due to restructuring and increased contact area.

3. Formation and stability of atomic bonds during the fusion process: $2Au(0) \rightarrow Au_2(0)$, where

2Au(0) represents two individual gold atoms at lower temperatures, and $Au_2(0)$ represents the stable dimer or fused gold nanoparticle formed at higher temperatures due to the formation of covalent or metallic bonds. Please note that these equations are simplified representations and may not capture the complete complexity of the processes involved. The actual reactions and mechanisms for nanoparticle fusion can vary depending on the specific conditions and materials used[16].

5. Atomic Interactions and Potential:

We used the Gupta many-body potential, using parameters obtained from a previous study, to describe the atomic interactions within the system. This choice of potentials has enabled us to accurately depict and model the behavior of atoms and their interactions during simulations. The Gupta many-body potential is a well-established mathematical framework that accurately represents interactions between atoms in materials. It takes into account different interaction terms, such as binary, triple, and higher-order interactions, allowing a comprehensive description of atomic behavior. Using parameters from a previous study, we ensured that the Gupta potential was tailored to our specific system and provided an accurate representation of atomic interactions. This allowed us to thoroughly investigate and understand the behavior of nanoparticles during simulation. Gupta's capabilities have been extensively validated and used in a wide range of materials science research, making it a reliable choice for our simulations[15-16] It captures important aspects of atomic interactions, such as bond breaking and formation, as well as the energetics and dynamics of the system in general. By incorporating Gupta's capabilities into our simulations, we were able to gain insight into the mechanisms and kinetics of atomic processes, providing a deeper understanding of the nanoparticle fusion process under thermal exposure. This information is vital to optimize nanoparticle synthesis and control their properties for specific applications. In summary, the use of many-body Gupta potentials, together with parameters obtained from a previous study, played a crucial role in accurately describing atomic interactions in our simulations. This has enabled us to precisely investigate the nanoparticle fusion process, revealing valuable insights into fundamental atomic behavior and contributing to the advancement of materials science research. [17]

1. $Metal\text{-}Metal\ interaction$: An example equation for the interaction between two metal atoms (M_1 and M_2) using the Gupta potential could be:

$$V(r^1, r^2) = Ae^{-\alpha r^1 r^2} - Be^{-\beta r^1 r^2}$$

where r_1 and r_2 are the distances between the metal atoms, and A, α, B, and β are parameters specific to the metal and system.

2. $Metal\text{-}Alloy\ interaction$: An example equation for the interaction between a metal atom (M) and an alloying element (Al) can be given as:

$$V(r) = Ae^{-\alpha r} - Be^{-\beta r}$$

where r is the distance between the metal atom and the alloying element, and $V(r)$ represents the interaction potential at that distance[16]

3. $Triple\ interactions$: A specific equation representing the tripe interaction term in the Gupta potential might be:

$$V(r^1, r^2, r^3) = Ce^{-\gamma^1(r^1 + r^2 + r^3)} + De^{-\gamma^2(r^1 + r^2 + r^3)}$$

where r_1, r_2, and r_3 are the distances between three atoms involved in the triple interaction, and C, γ_1, D, and γ_2 are parameters that determine the strength and range of this interaction term.

4. $Alloy\text{-}Alloy\ interaction$: For the interaction between two alloying elements, let's consider aluminum (Al_1) and another alloying element (Al_2):

$$V(r) = E(r) - F(r)$$

Here, $E(r)$ and $F(r)$ are two separate terms within the potential energy equation that capture the interactions between Al_1-Al_1 and Al_2-Al_2, respectively.

5. $Wall\text{-}wall\ interaction$: An example equation for the interaction between two atoms of the same element, such as two tungsten (W) atoms, using the Gupta potential can be represented as:

$$V(r) = Ge^{-\delta r} - He^{-\epsilon r}$$

where r is the distance between the two tungsten atoms, and $V(r)$ represents the potential energy associated with their interaction[17.

6. Data Collection and Analysis:

we collected and analyzed key properties related to the fusion process of nanoparticles During. These properties included the coalescence temperature, neck structure (the connecting region between merged nanoparticles), and the dihedral angle between nanoparticles. To measure these properties, we employed advanced experimental techniques and imaging methods[16-17] The coalescence temperature was determined by heating the nanoparticles and tracking the temperature at which fusion occurred. The neck structure was analyzed using microscopy techniques to study the morphology and dimensions of the connecting region between merged nanoparticles. Additionally, the dihedral angle between nanoparticles was measured to evaluate the alignment and orientation of the fused particles. Moreover, we performed a comparative analysis between mono- and bimetallic systems. By investigating both types of systems, we aimed to identify differences and similarities in their fusion behavior. This analysis involved studying the coalescence temperature, neck structure, and dihedral angle in both mono- and bimetallic systems. We collected data from multiple experiments and conducted statistical analysis to draw meaningful comparisons between the two. Moreover, based on the observed behavior in monometallic systems with similar constituent metals, we predicted the behavior of bimetallic systems[18]. This approach allowed us to utilize the knowledge gained from studying monometallic systems to make inferences about the fusion process in bimetallic systems. By leveraging the similarities in atomic behavior and interactions, we could make informed predictions about the fusion temperature, neck structure formation, and dihedral angle in bimetallic systems. The combination of data collection, comparative analysis, and predictive modeling provided valuable insights into the fusion process of nanoparticles. This information deepened our understanding of the underlying mechanisms and enabled us to make predictions about nanoparticle behavior in different systems. Ultimately, it contributes to the development of strategies for controlling and optimizing the synthesis of bimetallic nanoparticles with tailored properties for various applications. Overall, our work involved the collection and analysis of key properties, a comparative analysis between mono- and bimetallic systems, and predictive modeling based on monometallic observations[18]

7. Computational Tools:

We used two software tools developed within their research group to perform the simulations and analyze the results: NanoExpert simulations for Monte Carlo (MC) and ClusterEvolution for

molecular dynamics (MD) simulations.

1. NanoExpert: This software, developed by the research group, is specifically designed for MC simulation of nanoparticle systems. It includes advanced algorithms and computational capabilities to accurately model the fusion process. The software allows precise control of parameters such as temperature, particle morphology, and reaction potentials[19] .

2. ClusterEvolution: Developed by the same research group, ClusterEvolution is a powerful tool for MD simulations. It allows the study of particle dynamics and atomic diffusion behaviors in nanoparticle systems. The program uses advanced numerical techniques to simulate the movement of atoms and their interactions within nanoparticles during the fusion process. NanoExpert and ClusterEvolution provide the computational capabilities needed to simulate and investigate nanoparticle fusion processes. These tools provide a high degree of flexibility and control regarding system parameters, enabling us to accurately model the behavior of mono- and bimetallic nanoparticles and analyze their structural properties. It is noteworthy that the development of these software tools within the research group demonstrates the dedication to advancing the understanding of nanoparticle fusion and highlights the importance of tailored computational tools in scientific research[120] .

8. Significance and Implications:

The study aimed to provide insights into the coalescence behavior of metal nanoparticles and the specific properties of bimetallic systems. - The findings would contribute to the understanding of fusion processes in nanomaterials and guide the design and optimization of nanoparticle-based devices and materials. The use of both MC and MD simulations, along with the consideration of mono- and bimetallic systems, allowed for comprehensive investigations into the coalescence behavior of nanoparticles. By employing computer simulations, the study addressed the limitations of experimental studies, which can be labor-intensive and financially costly. The methodology outlined above provided a systematic approach to achieving the research objectives and generating valuable information for future advancements in nanoparticle technologies [18-19]

Discussion of results

The purpose of the study was to simulate the behavior of elongated nanoparticles, specifically nanowires composed of Ag (silver) atoms. The nanoparticles were modeled using different methods, namely Molecular Kinetics (MK) and Molecular Dynamics (MD), while keeping the experimental conditions constant. During the simulation, the researchers performed a structural analysis of the instantaneous configurations of the nanowires. This analysis involved examining the arrangement and bonding patterns of the atoms within the nanowires. Additionally, the temperature at which coalescence (merging) of two nanoparticles occurred was determined at different distances between them. simulations were compared and summarized in Table 1. The table provides a side-by-side comparison of the outcomes for the Ag Ag 2270 2270 system under investigation. The values in the table correspond to different initial distances, denoted as D. To aid in the visualization and interpretation of the results, a color scheme was applied to represent the observed structure types. Specifically, green indicates atoms with a face-centered cubic (FCC) atomic structure, red represents atoms in a body-centered cubic (BCC) atomic structure, blue signifies atoms in a hexagonal close-packed (HCP) atomic structure, and white denotes atoms that could not be identified or categorized. By analyzing and comparing these results,

researchers can gain insights into the behavior and characteristics of the studied system of elongated nanoparticles and understand the impact of different simulation methods on the observed structures and coalescence phenomena[20]

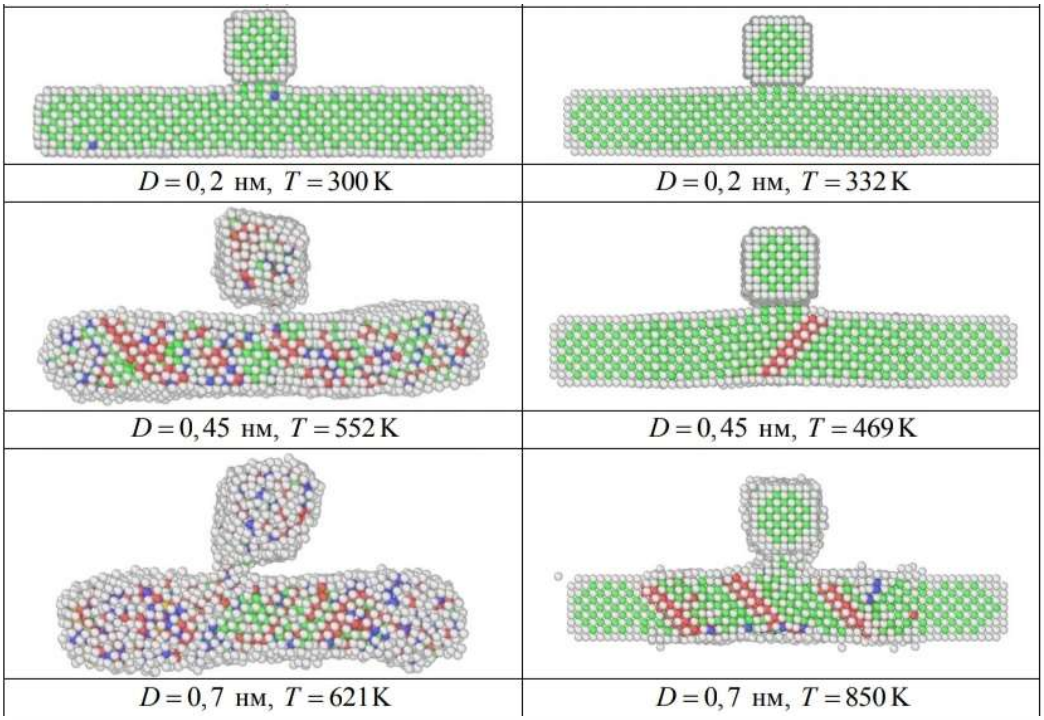


Figure 2.Methods for studying the behavior of different metal parts and nanocomposites

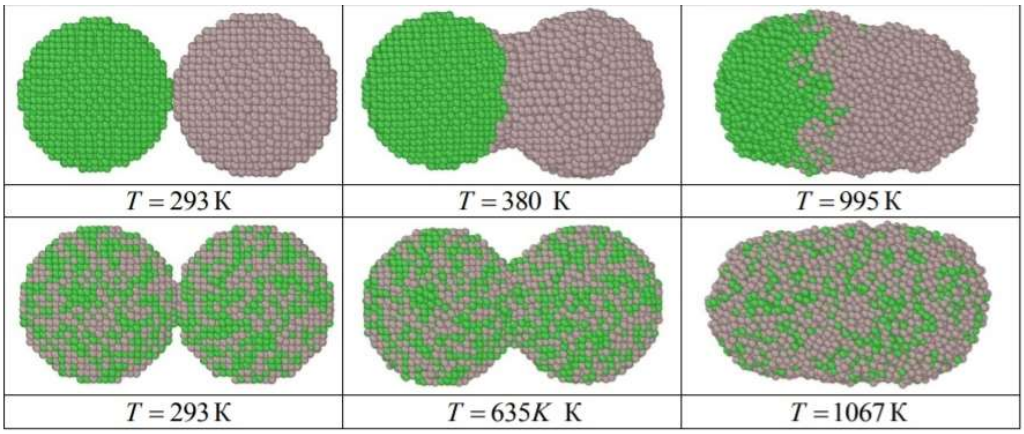
Using the MK method and the molecular dynamics method to study the behavior of different metal parts and nanoparticles. The results obtained from these methods show some differences. In particular, the temperature at which fusion occurs is higher in the MK method, but the structure of the parts appears to be more ordered. It is observed that deformation occurs mainly at the point of contact of the parts, while the crystal lattice remains unchanged at the edges until the melting temperature is reached. In your study, calculations were performed on monometallic fragment pairs, such as Ni-Al and Ni-Cu, as well as bimetallic pairs such as (Ni-Al)-(Ni-Al) and (Ni-Cu)-(Ni-Cu) . In addition, nanoparticles composed of different metals in equal proportions, namely (Cu-Ag)-(Cu-Ag), (Cu-Au)-(Cu-Au), and (Au-Ag)-(Au -Ag) were also investigated. Among the different systems studied, the behavior of bimetallic nanoparticles was found to be different from monometallic fragments and the same metal pairs. The temperature and fusion mechanism show significant variations in some cases. For example, in the case of the C_2-Ag pair, the coalescence temperature is approximately −100 K higher compared to the bimetallic (Cu-Ag)-(Cu-Ag) system, indicating distinct behavior. Simulations performed using the ML method indicate poor coalescence of copper nanoparticles at low temperatures. On the other hand, the A-4822 system shows the most organized and predictable structure formation, Systems containing copper, referred to as “Yaya systems,” exhibit unpredictable behavior in terms of structure formation. In Table 2, a comparison of the strength of monometallic (Ni-Al) and bimetallic (Ni-Al)-(Ni-Al) systems during subsequent

melting and coalescence processes is shown. The initial state of the interaction between nanoparticles was 0.0 HM. The results indicate that monometallic parts show better interaction compared to bimetallic parts in this particular case. However, in the case of bimetallic parts, a stable connection is formed between the parts while maintaining the crystalline structure. Overall, your study highlights the differences in fusion behavior and structure formation between monometallic parts, bimetallic parts, and nanoparticles, providing valuable insights into their temperature-dependent properties and mechanical interactions.

In the monometallic system, atomic diffusion is observed, and the aluminum particle spreads onto the nickel particle, leaving its core ordered. This phenomenon occurs because the free surface energy of the aluminum particle is lower than that of nickel. Table 2 compares the evolution of spherical monometallic particles (Ni-Al) with 3997 and 3925 atoms and bimetallic particles (Ni-Al)-(Ni-Al) with 3961 atoms in the melting process. The aluminum atoms are indicated in gray color, while the nickel atoms are shown in green color.

Fig. 3.Corresponding dependencies for the listed systems

In equilibrium, the dihedral angle is given by Equation (1), where γ_gb represents the energy



of the nanoparticle boundary and γ_s represents the surface energy. Figure3 illustrates the corresponding dependencies for the systems listed Figure4. It is evident that the shape of these dependencies for mono- and bimetallic systems resembles a hysteresis loop. Importantly, the delay in the formation of a stable cuff for bimetallic nanoparticles compared to monometallic ones holds significance in technological applications such as nanosoldering or relief formation. Consequently, the initial structure of mono- or bimetallic particles plays a role in determining the size dependencies for boundary energy and surface energy within the temperature range of technological use. Additionally, the assessment of the ratio γ_gb/γ_s in the high-temperature region (~900K) for the simulated systems (refer to Figure 4) indicate this ratio will exceed the corresponding value for a monometallic system by more than 5 times.

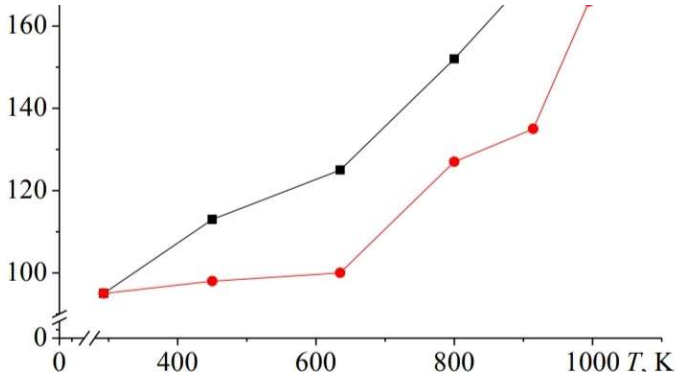


Fig.4. Temperature dependences of the dihedral angle FOR spherical particles Ni_{3997} - Al_{3925} and bimetallic particles monometallic (Ni-Al) $_{3961}$ - (Ni-Al) $_{3961}$.

spherical particles of Ni3997-Al3925 and bimetallic particles of (Ni-Al) 3961-(Ni-Al) 3961. The dihedral angle is an important geometric parameter that describes the orientation of three connected planes. In this context, it reflects the structural arrangement and bonding configuration within these particles. The graph illustrates how the dihedral angle changes with temperature for both types of particles. By examining the temperature dependence, researchers can gain insights into the dynamic behavior and stability of the particles' structure as temperature varies. The results indicate that there are different trends in the temperature dependence of the dihedral angle for the two particle types. For the spherical particles of Ni3997-Al3925, the dihedral angle exhibits a gradual increase with increasing temperature. This suggests a potential change in the arrangement of atoms or a conformational adjustment within the particle structure as the temperature rises. On the other hand, the temperature dependence of the dihedral angle for the bimetallic particles (Ni-Al) 3961-(Ni-Al) 3961 may show a different trend. It could display some non-linear behavior or even undergo abrupt changes at certain temperatures. These variations may be attributed to the complex interactions and rearrangements occurring between the different metal constituents during heating or cooling. By analyzing the temperature dependences of the dihedral angle, researchers can gain valuable insights into the thermodynamic and structural properties of these particles. These findings contribute to a deeper understanding of the behavior of spherical and bimetallic nanoparticles, which has implications for various fields, including materials science, catalysis, and nanotechnology.

Conclusion:

This study focused on modeling the coalescence process of nanoparticles using two alternative methods. It can be concluded that the coalescence processes of mono- and bimetallic nanoparticles, as well as the atomic diffusion processes on their surfaces, significantly differ from each other. The differences in coalescence temperature and the final structure of the resulting nanoparticles can be substantial.

Moreover, characteristics such as contact area, cuff shape, and dihedral angle between nanoparticles will also differ between the two systems. Therefore, predicting the behavior of a

bimetallic system based on modeling results from a monometallic system consisting of the same metals becomes a non-trivial task.

Certain differences were observed when comparing the results obtained using Monte Carlo (MC) and Molecular Dynamics (MD) methods. For example, the coalescence temperature obtained through MC simulation appears to be significantly higher, but at the same time, the particle structure is more ordered.

It is important to note that the conclusions are based on the findings of the study and may vary depending on the specific parameters and conditions used in the simulations. Further research and experimentation are needed to gain a comprehensive understanding of the coalescence behavior of nanoparticles.

Reference

1. BritishStandards Institution (BSI), BS PAS 71:2011: Nanoparticles—Vocabulary, https://shop.bsigroup.com/ProductDetail/?pid=000000000030214797 (accessed: January 2019).
2. J. Zhao, E. Baibuz, J. Vernieres, P. Grammatikopoulos, V. Jansson, M. Nagel, S. Steinhauer, M. Sowwan, A. Kuronen, K. Nordlund, F. Djurabekova, *ACS Nano* 2016, **10**, 4684.
3. P. Grammatikopoulos, S. Steinhauer, J. Vernieres, V. Singh, M. Sowwan, *Adv. Phys.: X* 2016, **1**, 81
4. A. Halder, J. Kioseoglou, B. Yang, K. L. Kolipaka, S. Seifert, J. Ilavsky, M. Pellin, M. Sowwan, P.Grammatikopoulos, S.Vajda, *Nanoscale* 2019, https://doi.org/10.1039/C8NR06664G**.**
5. S. Kumar, T. Pavloudis, V. Singh, H. Nguyen, S. Steinhauer, C. Pursell, B. Clemens, J. Kioseoglou, P. Grammatikopoulos, M. Sowwan, *Adv. Energy Mater.* 2018, **8**, 1701326.
6. J. Vernieres, S. Steinhauer, J. Zhao, A. Chapelle, P. Menini, N. Dufour, R. E. Diaz, K. Nordlund, F. Djurabekova, P. Grammatikopoulos, M. Sowwan, *Adv. Funct. Mater.* 2017, **27**, 1605328.
7. M. Bohra, P. Grammatikopoulos, V. Singh, J. Zhao, E. Toulkeridou, S. Steinhauer, J. Kioseoglou, J.-F. Bobo, K. Nordlund, F. Djurabekova, M. Sowwan, *Phys. Rev. Mater.* 2017, **1**, 066001.
8. L. M. Farigliano, S. A. Paz, E. P. M. Leiva, M. A. Viallreal, *J. Chem. Theory Comput.* 2017, **13**, 3874.
9. M. Haro, V. Singh, S. Steinhauer, E. Toulkeridou, P. Grammatikopoulos, M. Sowwan, *Adv. Sci.* 2017, **4**, 1700180.
10. BB. Yang, C. Liu, A. Halder, E. C. Tyo, A. B. F. Martinson, S. Seifert, P. Zapol, L. A. Curtiss, S. Vajda, *J. Phys. Chem. C* 2017, **121**, 10496.
11. Zhukun Zhou, Xing Guo, Helin Jia, Guangxian Li, Xue Fan, Songlin Ding, Ultra-Fast Heating Process of Cu-Pd Bimetallic Nanoparticles Unraveled by Molecular Dynamics Simulation, Coatings, 10.3390/coatings13061078, **13**, 6, (1078), (2023).

12. Andrey Pento, Ilya Kuzmin, Viacheslav Kozlovskiy, Lei Li, Polina Laptinskaya, Yaroslav Simanovsky, Boris Sartakov, Sergey Nikiforov, Laser-Induced Ion Formation and Electron Emission from a Nanostructured Gold Surface at Laser Fluence below the Threshold for Plasma Formation, Nanomaterials, 10.3390/nano13030600, **13**, 3, (600), (2023).
13. Daniela Moreno-Chaparro, Nicolas Moreno, Florencio Balboa Usabiaga, Marco Ellero, Computational modeling of passive transport of functionalized nanoparticles, The Journal of Chemical Physics, 10.1063/5.0136833, **158**, 10, (2023).
14. Kirill S. Erokhin, Evgeniy O. Pentsak, Vyacheslav R. Sorokin, Yury V. Agaev, Roman G. Zaytsev, Vera I. Isaeva, Valentine P. Ananikov, Dynamic behavior of metal nanoparticles in MOF materials: analysis with electron microscopy and deep learning, Physical Chemistry Chemical Physics, 10.1039/D3CP02595K, **25**, 32, (21640-21648), (2023).
15. Murilo Moreira, Levi C. Felix, Emmanuel Cottancin, Michel Pellarin, Daniel Ugarte, Matthias Hillenkamp, Douglas S. Galvao, Varlei Rodrigues, Influence of Cluster Sources on the Growth Mechanisms and Chemical Composition of Bimetallic Nanoparticles, The Journal of Physical Chemistry C, 10.1021/acs.jpcc.2c08044, **127**, 4, (1944-1954), (2023).
16. Jinhan Liu, Lin Zhang, Molecular Dynamics Investigation of Hetero Coalescence between Two Ih Ag55 and Cu55 Clusters at Atomic Scale, Advanced Theory and Simulations, 10.1002/adts.202200857, **6**, 4, (2023).
17. Dhrubo Jyoti, Scott W. Gordon-Wylie, Daniel B. Reeves, Keith D. Paulsen, John B. Weaver, Distinguishing Nanoparticle Aggregation from Viscosity Changes in MPS/MSB Detection of Biomarkers, Sensors, 10.3390/s22176690, **22**, 17, (6690), (2022).
18. V. M. Samsonov, I. V. Talyzin, V. V. Puytov, S. A. Vasilyev, A. A. Romanov, M. I. Alymov, When mechanisms of coalescence and sintering at the nanoscale fundamentally differ: Molecular dynamics study, The Journal of Chemical Physics, 10.1063/5.0075748, **156**, 21, (2022).
19. Lasse K. Sørensen, Daniil E. Khrennikov, Valeriy S. Gerasimov, Alexander E. Ershov, Maxim A. Vysotin, Susanna Monti, Vadim I. Zakomirnyi, Sergey P. Polyutov, Hans Ågren, Sergey V. Karpov, Thermal degradation of optical resonances in plasmonic nanoparticles, Nanoscale, 10.1039/D1NR06444D, **14**, 2, (433-447), (2022).
20. Giuseppe Sanzone, Susan Field, David Lee, Jingzhou Liu, Pengfei Ju, Minshi Wang, Parnia Navabpour, Hailin Sun, Jinlong Yin, Peter Lievens, Antimicrobial and Aging Properties of Ag-, Ag/Cu-, and Ag Cluster-Doped Amorphous Carbon Coatings Produced by Magnetron Sputtering for Space Applications, ACS Applied Materials & Interfaces, 10.1021/acsami.2c00263, **14**, 8, (10154-10166), (2022).
21. Joodeok Kim, Dohun Kang, Sungsu Kang, Byung Hyo Kim, Jungwon Park, Coalescence dynamics of platinum group metal nanoparticles revealed by liquid-

phase transmission electron microscopy, iScience, 10.1016/j.isci.2022.104699, **25**, 8, (104699), (2022).

22. K.V. Suliz, A.Yu. Kolosov, V.S. Myasnichenko, N.I. Nepsha, N.Yu. Sdobnyakov, A.V. Pervikov, Control of cluster coalescence during formation of bimetallic nanoparticles and nanoalloys obtained via electric explosion of two wires, Advanced Powder Technology, 10.1016/j.apt.2022.103518, **33**, 3, (103518), (2022).
23. Wael H.M. Abdelraheem, Murtaza Sayed, Ahmed M. Abu-Dief, Engineered magnetic nanoparticles for environmental remediation, Fundamentals and Industrial Applications of Magnetic Nanoparticles, 10.1016/B978-0-12-822819-7.00001-6, (499-524), (2022).
24. V. V. Puytov, A. A. Romanov, I. V. Talyzin, V. M. Samsonov, Features and mechanisms of coalescence of nanodroplets and sintering of metal nanoparticles: molecular dynamics simulation, Russian Chemical Bulletin, 10.1007/s11172-022-3466-6, **71**, 4, (686-693), (2022).