Proceedings of the 7th International Conference on Materials Chemistry and Environmental Engineering
DOI: 10.54254/2755-2721/2027.38611

Sintering of Metallic Core-Shell Nanoparticles: Molecular Dynamics Insights

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Abstract. Core-shell nanoparticles (CSNPs) have attracted considerable attention as interconnect materials for advanced electronic packaging. Their compositional and structural flexibility have enabled a balance among electrical and thermal conductivity, oxidation resistance, material cost, and low-temperature sinterability. This review summarizes recent progress in the sintering behavior and mechanical performance of CSNPs, with particular emphasis on atomic-scale mechanisms revealed by molecular dynamics (MD) simulations. The roles of core-shell interfaces, shell thickness, particle size, sintering temperature, external pressure, and processing atmosphere in atomic diffusion, neck formation, defect evolution, pore elimination, and densification are systematically discussed. Current limitations associated with simulation time and length scales and the accuracy of empirical potentials are discussed. Future developments are expected to involve machine-learning interatomic potentials, integrated modeling of MD, phase-field modeling, finite-element analysis, large-scale multiparticle simulations, and extension toward compositionally complex and high-entropy alloy (HEA) NPs. These advances may provide a more reliable framework for understanding sintering mechanisms and guiding the rational design of high-performance nanoparticle interconnect materials.

Keywords: core-shell nanoparticles, nanoparticle sintering, molecular dynamics simulation, interfacial diffusion, mechanical properties

1. Introduction

Power devices, high-frequency devices, and flexible electronics place demanding requirements on the materials used for interconnection in advanced electronic packaging. Conductivity alone is insufficient: the materials must conduct both heat and electricity, allow bonding at low processing temperatures, and provide joints with high strength and long-term reliability [1-3]. Figure 1 provides an overview of the core-shell structure, sintering stages and atomic-scale mechanisms, key structural and processing parameters, MD simulation and analysis methods, and potential applications discussed in this review.

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DOI: 10.54254/2755-2721/2027.38611

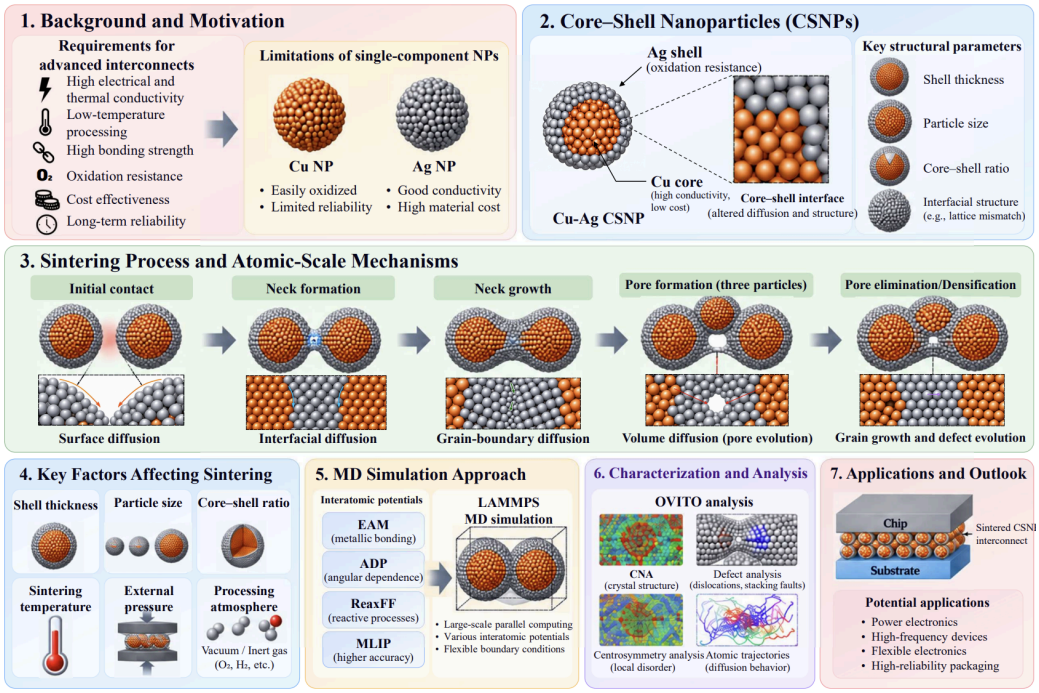

Figure 1. Schematic overview of the sintering behavior and molecular dynamics investigation of metallic core-shell nanoparticles

Sintering offers a way to join metallic nanoparticles (NPs) and has therefore received considerable research attention [1, 3-5]. Relative to bulk material, NPs have a larger specific surface area and higher surface free energy. These properties favor atomic migration and coalescence at relatively low temperatures, making bonding possible [4-6]. Thermally activated atomic motion and attraction between neighboring particles bring their surfaces into contact. Material then reaches the contact region through surface, grain-boundary, and volume diffusion, forming a neck between the particles. Continued transport enlarges the neck and can be followed by pore elimination and structural densification [4, 6-8].

The choice of a single metal involves practical limitations. Cu NPs are readily oxidized, while Ag and other noble-metal NPs offer excellent electrical and thermal conductivity at a higher material cost [2, 9, 10]. These limitations can constrain both the reliability and the economic viability of NP interconnects. Research on particle structure and composition seeks to address this combination of constraints [2, 10, 11].

An inner core enclosed by an outer shell defines the core-shell nanoparticle (CSNP) structure [2, 9, 10, 12]. The two regions can serve different purposes. A lower-cost core can supply useful electrical and thermal properties, while the shell can improve surface stability and resistance to oxidation [2, 9, 10]. The interface between them also changes the structure of the particle. Atomic diffusion, crystal-structure evolution, and sintering kinetics can differ in this region from those elsewhere in the particle [9, 10, 12]. Control of the interface and of the core-shell geometry therefore provides a means of regulating sintering behavior.

Shell thickness, overall particle size, the core-to-shell size ratio, and the state of the interface all influence atomic migration and microstructural evolution during sintering [2, 9, 12, 13]. Their effects are evident in MD studies of Cu-Ag CSNPs. Changing the shell thickness alters surface and interfacial diffusion, lattice mismatch, and the developing neck structure [9, 12, 14, 15]. A suitable

DOI: 10.54254/2755-2721/2027.38611

shell structure can facilitate atomic motion and neck growth, assist pore elimination and densification, and thereby affect bonding and mechanical performance [2, 9, 10]. Understanding how these responses depend on particle geometry is necessary for selecting NP joining conditions.

The core-shell architecture also affects which defects form during sintering and how they evolve. MD studies have identified dislocations, stacking faults, grain boundaries, amorphous regions, and other defects that modify diffusion paths and local atomic rearrangements [7, 9, 12, 16]. Changes in these defects can influence densification and the mechanical response of the sintered material [2, 3, 10]. Interfacial evolution and defect evolution thus need to be considered together when assessing the reliability of a CSNP interconnect.

Both experiments and simulations have been used extensively to study NP sintering. In situ transmission electron microscopy can reveal changes in particle shape, neck size, and particle rotation, whereas MD resolves the underlying atomic motion [17]. Combining these approaches allows observed sintering behavior to be interpreted using atomistic mechanisms [17, 18]. MD simulations have been widely used to investigate atomic diffusion, defect evolution, and pressure-assisted sintering [1-3, 7, 9]. Other studies have examined how shell structure, particle size, crystallographic misorientation, temperature, and the choice of interatomic potential affect sintering behavior and simulation results [12, 13, 16, 19, 20]. This review examines research published in 2010-2026 on CSNP sintering and mechanical strength, with an emphasis on MD results. It considers how particle geometry, interfacial characteristics, and processing conditions affect transport, microstructural evolution, densification, and mechanical performance.

2. Fundamentals of CSNP sintering

2.1. Structural characteristics and interfacial features

The core-shell interface plays an important role in determining sintering behavior. Differences in lattice structure and atomic arrangement between the core and shell can produce interfacial mismatch and local structural disorder, which may affect atomic mobility, crystallization, and defect evolution during sintering [9, 12]. Therefore, the sintering behavior of CSNPs is governed not only by the free surface but also by the structural characteristics of the core-shell interface.

2.2. Surface energy, size effects, and melting-point depression

Reducing particle size increases the relative importance of the surface. Atomic mobility is generally enhanced, allowing NPs to sinter at temperatures well below those needed for bulk material [4, 6]. MD simulations show that size also affects neck evolution, diffusion, and the microstructure that develops during sintering [6, 13]. In a CSNP, these effects are coupled with shell thickness and interfacial structure. Their interaction gives rise to thermal and diffusion behavior that is more complex than in a particle made from a single metal [9, 12].

Melting-point depression provides another example of the increased surface contribution at small particle sizes. Van Teijlingen et al. measured Ni NPs approximately 3-6 nm in diameter and found a substantial decrease in melting temperature as diameter decreased [21]. Figure 2 compares the measurements with MD and thermodynamic predictions, which show the same strong dependence on size. The particles in that study were monometallic Ni, so the results do not directly describe a core-shell system. They nevertheless illustrate the size-dependent thermal behavior of metallic NPs and help explain the enhanced thermal activity of nanoscale core-shell structures.

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2.3. Sintering process of CSNPs

NP sintering can generally be described as a continuous process involving initial particle contact, sintering-neck formation, neck growth, and pore elimination accompanied by densification [4-6]. When two NPs come into contact, the high-energy atoms near the contact region undergo rearrangement, creating an initial connection between the particles. With continued atomic migration, material accumulates around the contact region and a sintering neck gradually forms.

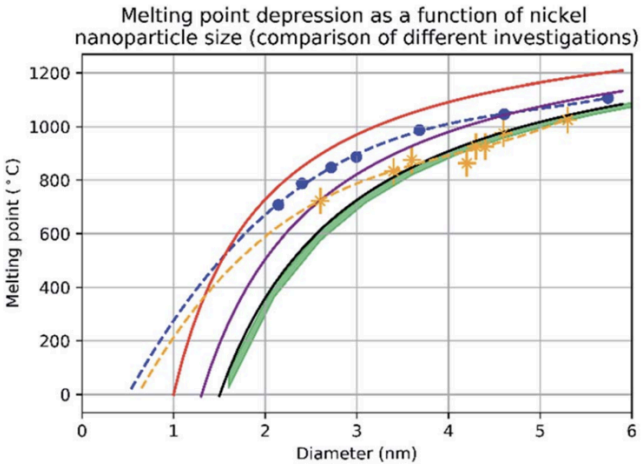

Figure 2. Size-dependent melting-point depression of Ni NPs obtained from experimental measurements and theoretical predictions. Reproduced from van Teijlingen et al. [21], Figure 4, published by the Royal Society of Chemistry. Licensed under the Creative Commons Attribution 3.0 Unported License (https://creativecommons.org/licenses/by/3.0/). Source: https://pubs.rsc.org/en/content/articlelanding/2020/na/d0na00153h.

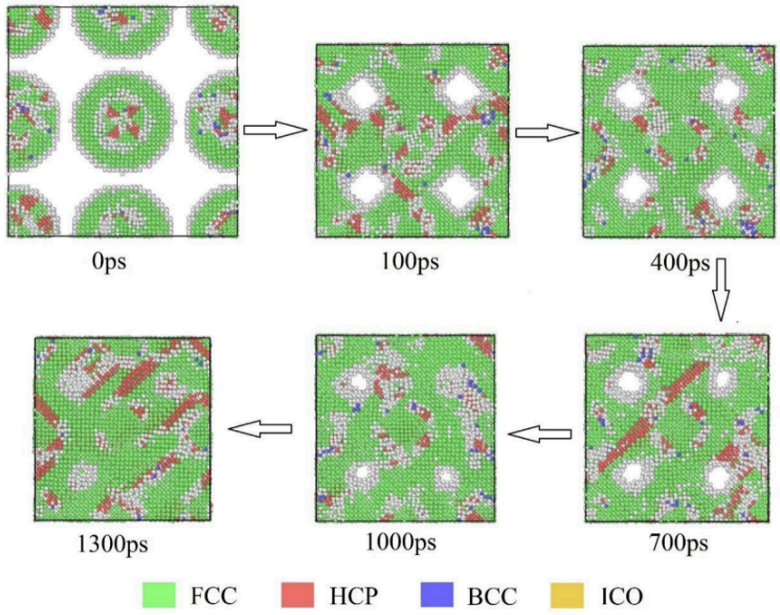

Figure 3. Microstructural evolution of Ag6Cu3 CSNPs during sintering characterized by common neighbor analysis (CNA). Reproduced from Zhang et al. [2], Figure 5. © 2026 by the authors. Licensed under the Creative Commons Attribution 4.0 International License (https://creativecommons.org/licenses/by/4.0/). Source: https://doi.org/10.3390/ma19081612

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During subsequent sintering, the neck continues to grow as atoms are transported through mechanisms including surface diffusion, grain-boundary or interfacial diffusion, and volume diffusion [4, 6]. At the nanoscale, plastic deformation and local structural rearrangement may also contribute to neck development [5, 9]. The atomic-scale evolution of this process can be directly visualized by MD simulations. As shown in Fig. 3, Zhang et al. [2] observed the gradual formation of interparticle necks, followed by neck enlargement and the development of a continuous interparticle network as sintering proceeded. As the neck expands, the distance between neighboring particle centers decreases and the remaining pores are gradually reduced, leading to increased structural densification.

For CSNPs, the process is more complex because both surface atoms and atoms near the core-shell interface can participate in mass transport. Studies on Cu-Ag CSNPs have shown that shell thickness can alter surface diffusivity, interfacial diffusion, crystallization behavior, and the atomic composition of the neck region [9, 12]. In multi-particle systems, highly mobile interfacial atoms can also contribute to densification and the formation of mechanically stronger sintered structures [10].

3. Sintering mechanisms of CSNPs

3.1. Interfacial atomic migration and diffusion

The core-shell interface introduces an additional pathway for atomic migration that is absent in single-component NPs. Local lattice mismatch and interfacial energy can modify atomic mobility and diffusion behavior near the interface [9, 12]. MD simulations of Cu-Ag CSNPs have shown that interfacial atoms can exhibit high mobility and contribute significantly to densification [10]. Although the sintering neck may initially consist mainly of shell atoms, atoms near the Cu-Ag interface can also participate in mass transport, particularly at elevated temperatures [9, 12]. Therefore, interfacial diffusion and interdiffusion between the core and shell are important factors governing structural evolution during CSNP sintering [9, 10, 12, 15].

3.2. Regulation of the core by the shell structure

In Cu-Ag NPs, the Ag shell limits oxidation of the Cu core and changes the rates and paths of surface and interfacial transport [22, 23]. MD results indicate that a thinner Ag shell can increase surface-atom mobility. If the shell becomes excessively thin, however, greater lattice mismatch and structural disorder may impede crystallization [9, 12]. Experiments show that heating can also cause Ag-shell dewetting, pre-melting, and pre-wetting, which facilitate contact and neck formation [22, 23]. Shell design therefore requires a balance between surface protection and stability, atomic mobility, and interfacial mismatch [9, 12, 22, 23].

3.3. Surface, grain-boundary, and volume diffusion

Atomic diffusion during sintering can proceed via surface, grain-boundary, interfacial, and volume diffusion [4-7]. Surface atoms are relatively mobile, making surface diffusion an important route for early neck formation [4, 5]. A growing neck does not, by itself, establish that substantial densification has occurred: surface diffusion alone may produce little densification, while grain-boundary and interfacial diffusion provide further transport routes [6, 7, 9]. Raising the temperature increases diffusivity and can make transport from deeper within the particle more important [9, 20].

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The contribution of each route consequently depends on the temperature, particle structure, and interfacial state [7-9].

3.4. Effect of structural defects

Defect formation changes the routes available for atomic transport and the way local stresses are accommodated during sintering. Vacancies, dislocations, stacking faults, grain boundaries, and twin boundaries can provide diffusion paths or accommodate local stress [14] and lattice mismatch [7, 12, 16]. In Cu-Ag CSNPs, dislocation emission from loops can assist crystal reconstruction. Shell thickness and particle size also affect defect formation and stability [12]. Grain boundaries, amorphous regions, and stacking faults near the neck can take part in plastic deformation and atomic rearrangement [7, 9, 15, 16]. These links connect defect evolution with diffusion, crystallization, densification, and the mechanical properties of the sintered structure [2, 7, 10, 12].

3.5. Sintering-neck growth and interfacial bonding

A neck between neighboring NPs is the clearest structural indication that bonding has begun. Mobile atoms first form a small connection at the contact region. Diffusion, local rearrangement, particle rotation, and plastic deformation then contribute to its growth [5, 6, 14, 15]. In Cu-Ag CSNPs, Ag shell atoms can dominate the initial neck, while subsequent interfacial diffusion and structural reconstruction strengthen the connection [9, 12, 22]. Tian et al. observed pre-melting and pre-wetting of Ag NPs, followed by Ag-dominated neck formation in Cu-Ag CSNPs [22]. SEM observations provide further evidence of neck growth and densification. In Fig. 4, the Cu-Ag particles are only partly connected below 230 °C; distinct sintering necks are visible in the SEM images at 230 °C [24]. Higher sintering temperatures produce more fusion and coarsening, less porosity, and a denser connected structure [24]. As the neck develops, the effective bonding area increases, contributing to densification and mechanical integrity [2, 10, 24].

4. Key factors affecting the sintering strength of CSNPs

4.1. Shell thickness

Shell thickness is one of the most important structural parameters controlling CSNP sintering. A reduction in shell thickness can increase the mobility of surface atoms and enhance the contribution of the core-shell interface to atomic transport [9, 12]. However, excessively thin Ag shells may generate stronger lattice mismatch and structural disorder, thereby suppressing crystallization and altering defect evolution [9, 12]. As shown in Fig. 5, shell thickness has a non-monotonic influence on mechanical performance, densification, and atomic mobility. Consequently, an appropriate shell thickness is required to balance atomic diffusion, densification, structural stability, and mechanical properties [2, 9, 12].

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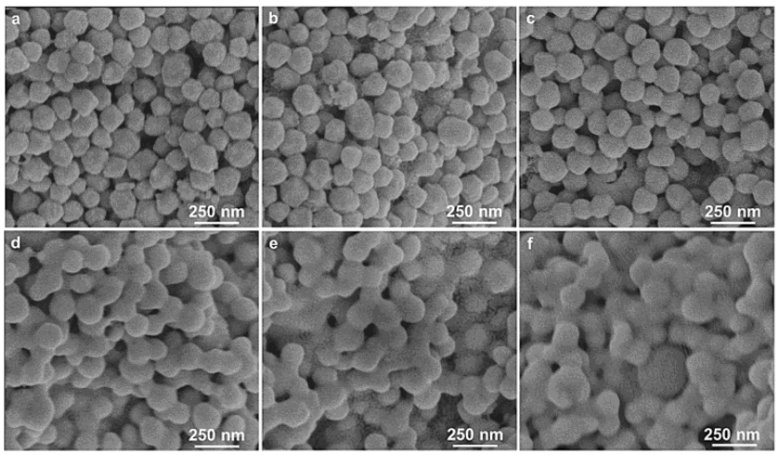

Figure 4. SEM images showing the temperature-dependent sintering evolution of Cu-Ag nanoparticle films at (a) 140 °C, (b) 170 °C, (c) 200 °C, (d) 230 °C, (e) 260 °C, and (f) 290 °C. Reproduced from Li et al. [24], Figure 6. © 2023 by the authors. Licensed under the Creative Commons Attribution 4.0 International License (https://creativecommons.org/licenses/by/4.0/). Source: https://doi.org/10.3390/mi14071318

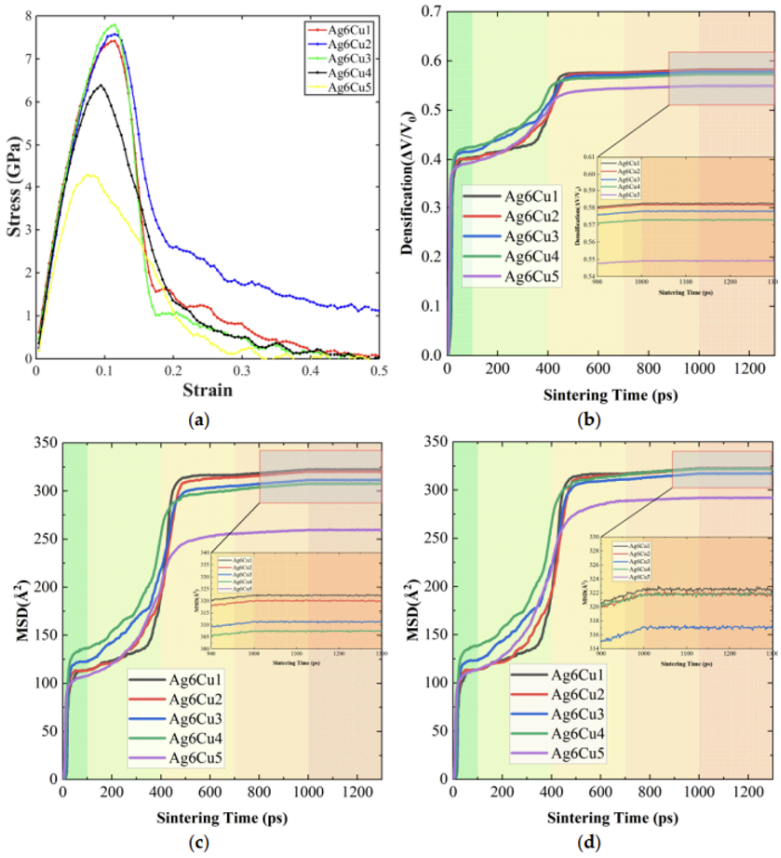

Figure 5. Effect of Ag shell thickness on the mechanical properties, densification, and atomic diffusion of Cu-Ag CSNPs. Reproduced from Zhang et al. [2], Figure 9. © 2026 by the authors. Licensed under the Creative Commons Attribution 4.0 International License (https://creativecommons.org/licenses/by/4.0/). Source: https://doi.org/10.3390/ma19081612

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4.2. Particle size

Smaller NPs generally have a stronger thermodynamic driving force for sintering because a larger fraction of their atoms lies near the surface. Their enhanced surface effects and atomic mobility can accelerate structural evolution [10, 13, 15]. For Cu-Ag CSNPs, size affects diffusion, defects, neck growth, densification, and the resulting mechanical properties [2, 10, 12]. The atomistic configurations in Fig. 6 illustrate differences in neck evolution, particle rotation, and structural rearrangement among metallic NPs of different diameters. These calculations concern monometallic Ag and Cu, rather than core-shell particles. They provide a useful reference for interpreting the general size effects relevant to CSNP sintering.

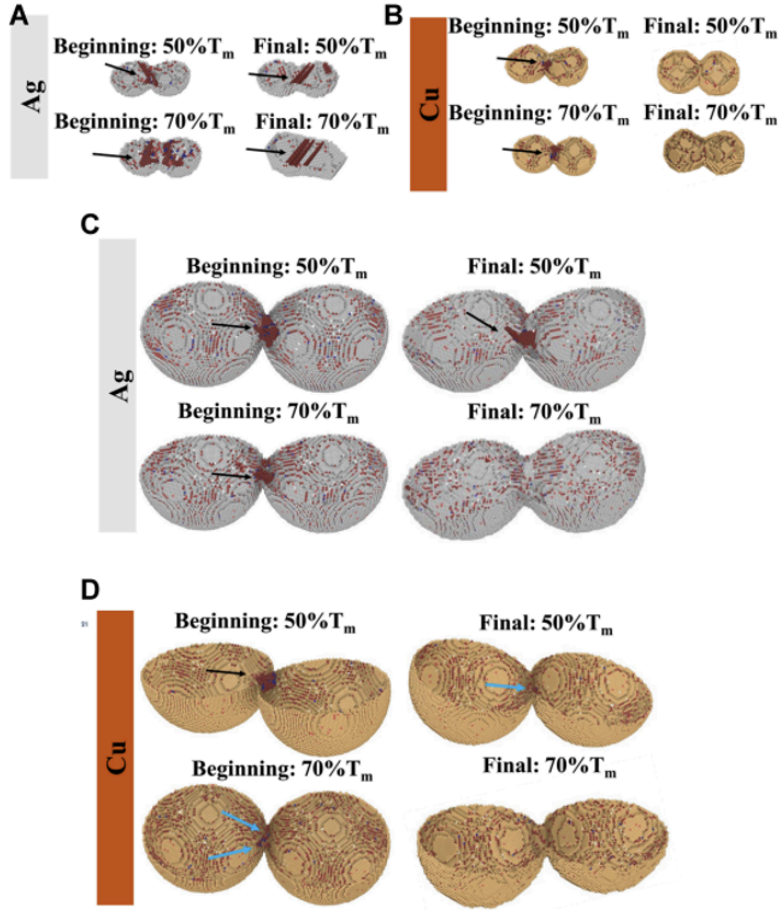

Figure 6. Representative atomistic configurations showing the size- and temperature-dependent defect evolution of Ag and Cu nanoparticles during sintering. Black arrows indicate dislocations, stacking faults, and twin boundaries, while light-blue arrows indicate vacancies. Reproduced from Jamshideasli et al. [7], Figure 3. © The Author(s) 2024. Licensed under the Creative Commons Attribution 4.0 International License (https://creativecommons.org/licenses/by/4.0/). Source: https://doi.org/10.20517/gmo.2024.062001

Nevertheless, smaller particles do not necessarily produce the highest mechanical strength because the final properties also depend on packing configuration, porosity, shell thickness, and microstructural defects [2, 10]. Therefore, particle size should be optimized together with the core-shell geometry rather than considered as an independent parameter [2, 12, 13].

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4.3. Sintering temperature

Sintering temperature has a direct influence on atomic mobility and mass transport. Increasing temperature generally enhances diffusion and accelerates neck growth, structural rearrangement, and pore elimination [2, 9, 12, 20]. At relatively low temperatures, surface diffusion and local structural rearrangement can dominate, whereas higher temperatures can activate stronger interfacial diffusion and even migration of Cu atoms toward the neck region [9, 12]. The influence of temperature on defect-mediated sintering is further illustrated in Fig. 7. At higher homologous temperatures, enhanced atomic mobility promotes more pronounced structural rearrangement and modifies the evolution of vacancies, dislocations, stacking faults, and twin boundaries in Ag and Cu nanoparticles [7]. Although these simulations involve monometallic nanoparticles, they provide useful insight into the temperature-dependent defect evolution relevant to CSNP sintering.

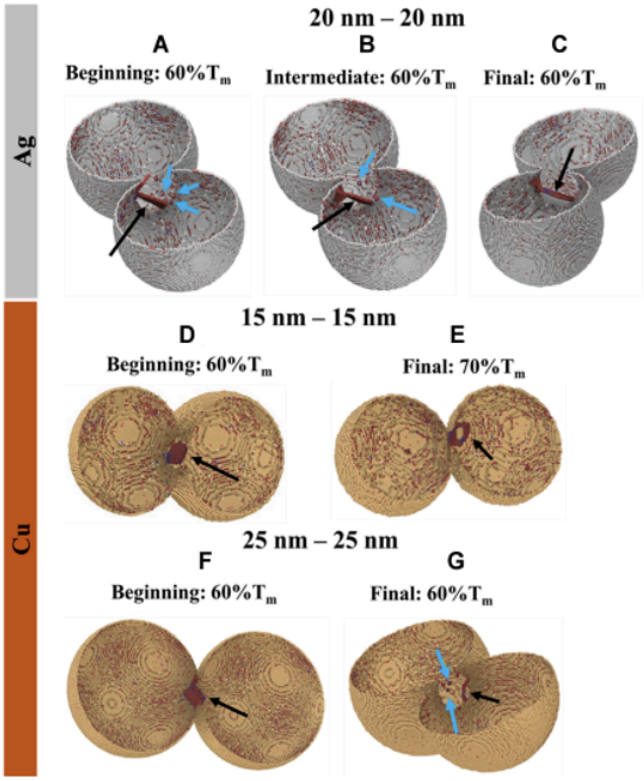

Figure 7. Representative atomistic configurations showing temperature-dependent defect evolution during the sintering of Ag and Cu nanoparticles. Black arrows indicate dislocations, stacking faults, and twin boundaries, while light-blue arrows indicate vacancies. Reproduced from Jamshideasli et al. [7], Figure 4. © The Author(s) 2024. Licensed under the Creative Commons Attribution 4.0 International License (https://creativecommons.org/licenses/by/4.0/). Source: https://doi.org/10.20517/gmo.2024.062001

Heating can induce Ag-shell dewetting or pre-wetting, and experiments link these changes to low-temperature sintering of Cu-Ag CSNPs [22, 23]. Excessively high temperatures may also change defect populations and microstructural stability. Selecting a sintering temperature therefore requires sufficient atomic mobility without compromising the stability of the sintered structure [2, 9, 12].

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4.4. External pressure

Applied pressure brings particles into closer contact, reduces gaps, and promotes rearrangement and plastic deformation, assisting densification [2, 3, 25]. MD studies of pressure-assisted Cu-Ag sintering show that increasing pressure can reduce porosity and promote neck growth and interfacial bonding [2, 25]. Kim and Chung found that Ag-coated Cu CSNPs undergo atomic migration and microstructural evolution that differ from those during conventional thermal sintering [25]. Pressure can thus change which mechanisms govern sintering, in addition to changing particle separation. The resulting mechanical properties reflect the combined effects of densification, diffusion, defects, and structural reconstruction under pressure [2, 25].

4.5. Sintering atmosphere and processing conditions

Oxidation is a particular concern when sintering Cu-containing NPs because a surface oxide can obstruct diffusion and bonding. Protective or reducing atmospheres can suppress oxidation. An Ag shell improves the oxidation resistance of the Cu core and allows Cu-Ag NPs to be sintered under less restrictive conditions [22, 23]. Tian et al. obtained Cu-Ag joints in ambient air at 250 °C with a shear strength of 26.5 MPa, showing how the shell can facilitate low-temperature bonding in air [22]. The heating method also matters. Ji et al. demonstrated ultrasonic-assisted sintering of Cu-Ag nanoparticle paste in air at temperatures as low as 160 °C. The optimized joints achieved a shear strength of 54.27 MPa at 180 °C [26]. Atmosphere, heating method, holding time, pressure, and auxiliary energy input together determine how far densification proceeds and the strength of the final joint [22, 23, 26].

5. MD simulations of CSNP sintering

5.1. Basic principles of MD simulation

MD simulation provides an atomistic approach for investigating NP sintering. Atomic trajectories are obtained by numerically integrating Newton's equations of motion, while interatomic potentials determine the forces between atoms [27, 28]. By tracking atomic positions, energies, mean-square displacement, local structures, and neck evolution, MD can reveal diffusion, defect evolution, interface reconstruction, and bonding processes that are difficult to resolve experimentally [2, 7, 9, 12, 13].

5.2. Packages and interatomic potentials

LAMMPS is an open-source package widely used for simulations of metallic NPs. Its parallel implementation, flexible boundary conditions, and range of interatomic potentials are useful for this work [27, 28]. Cu-Ag simulations commonly use embedded-atom method (EAM)-type potentials to describe metallic bonding [9, 12, 25]. The angular-dependent potential (ADP) extends this framework with angular-dependent interactions, permitting a more detailed treatment of local distortions and defect environments [29]. For reactive processes, the reactive force field (ReaxFF) uses a bond-order-dependent formulation to describe bond formation and dissociation [30]. Visualization and post-processing are often carried out in OVITO. Common-neighbor analysis, centrosymmetry analysis, and defect identification help quantify crystal structures and defects, including stacking faults and grain boundaries [31, 32].

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5.3. Mechanisms revealed by MD simulations

MD studies identify surface atoms and atoms near the core-shell interface as important contributors to transport during sintering. For Cu-Ag CSNPs, Ag shell atoms generally dominate early diffusion and neck formation; Cu atoms near the interface may become involved at higher temperatures or when the shell is thinner [9, 10, 12]. The simulations also resolve particle rotation, plastic deformation, defect formation, recrystallization, neck growth, and pore elimination directly [2, 7, 15, 16].

5.4. Simulation parameter design

Important structural variables include shell thickness, particle size, and the core-to-shell ratio [9, 12, 15]. Additional variables include sintering temperature, applied pressure, and the relative crystallographic orientation of the particles [2, 13, 25]. These parameters interact with each other and synergistically influence diffusion, defect evolution, densification, and mechanical properties. Therefore, future studies should increasingly consider multivariable parameter designs rather than isolated single-factor effects. The overall atomistic simulation workflow and its extension toward multiscale and compositionally complex systems are summarized in Fig. 8.

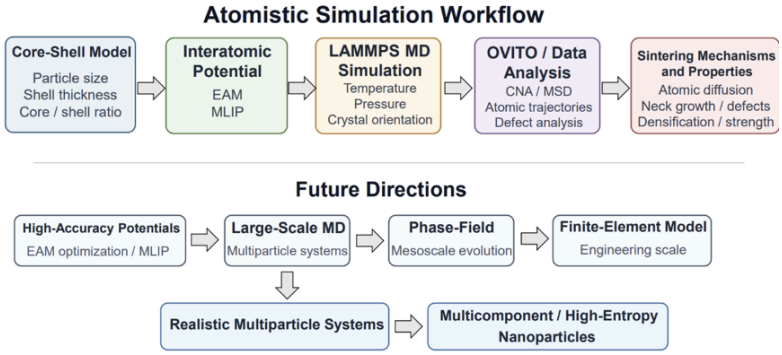

Figure 8. Schematic workflow of molecular dynamics simulation and future multiscale modeling strategies for core-shell nanoparticle sintering

6. Current challenges and future perspectives

6.1. Limitations of MD simulations

The main limitation of MD is its restricted time and length scales. Most simulations involve nanometer-scale systems and nanosecond-scale processes, whereas practical sintering occurs over much larger temporal and spatial ranges [27, 28]. Therefore, MD results should be carefully interpreted when applied to real processing conditions.

6.2. Development of more accurate interatomic potentials

The reliability of MD strongly depends on the interatomic potential. Classical empirical potentials are computationally efficient but may show limited transferability for complex interfaces, defect-rich structures, or multicomponent systems. Future potentials should more accurately describe surface energies, interface energies, stacking-fault energies, diffusion, and defect formation.

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Machine-learning interatomic potentials provide a promising balance between first-principles accuracy and classical MD efficiency [33, 34]. M3GNet, for example, uses graph neural networks to describe a broad range of chemical environments and enables large-scale atomistic simulations [34]. Such approaches may be particularly useful for complex core-shell and multicomponent systems.

6.3. Multiscale modeling

Multiscale coupling can bridge the gap between atomistic and engineering scales. MD can provide diffusion and interface parameters, while phase-field and finite-element method (FEM) simulations can describe longer-term microstructural evolution and macroscopic mechanical behavior [35, 36]. This MD-phase-field-FEM framework is therefore an important direction for future sintering studies.

6.4. Complex multicomponent and high-entropy alloy NPs

Future studies may extend binary metallic systems to multicomponent and high-entropy alloy (HEA) NPs. HEA NPs exhibit complex diffusion, segregation, lattice distortion, and defect behavior [37-39]. For example, CoCrCuFeNi NPs can develop core-shell-like structures due to Cu surface segregation and lattice-distortion-induced reconstruction [37]. FeNiCrCoAl NPs also show nanotwin formation, stacking faults, and dislocation activity [38].

Because conventional empirical potentials are difficult to construct for chemically complex HEAs, machine-learning potentials are especially attractive. Wu and Li demonstrated an ML interatomic potential (MLIP) for CrFeCoNiPd HEAs that reproduced atomic forces, lattice constants, stacking-fault energies, and dislocation behavior with good accuracy [40]. Combining MLIP with large-scale MD may therefore support future design of multicomponent, gradient-composition, and high-entropy NP interconnect materials.

7. Conclusion

CSNPs exhibit complex sintering behavior governed by the coupled effects of surface diffusion, interfacial diffusion, defect evolution, shell thickness, particle size, temperature, pressure, and processing conditions. In Cu-Ag systems, the Ag shell not only protects the Cu core from oxidation but also strongly influences atomic mobility, neck formation, crystallization, and densification. Meanwhile, the core-shell interface provides additional diffusion pathways and defect structures that can significantly affect the final bonding strength and mechanical properties.

MD simulations provide valuable atomic-scale insights into these processes by directly revealing atomic migration, interface reconstruction, defect evolution, and sintering-neck growth. However, limitations in simulation scale and interatomic potential accuracy remain important challenges. Future progress is expected to rely on more accurate MLIP, multiscale coupling of MD with phase-field and FEAs, and the extension of current models to more realistic multiparticle and multicomponent systems. In particular, HEA and compositionally complex NPs offer promising opportunities for developing advanced interconnect materials with tunable diffusion, interface, and mechanical properties. Overall, combining atomistic simulation with multiscale modeling and data-driven approaches will provide an increasingly powerful framework for the rational design and optimization of NP sintering processes.

DOI: 10.54254/2755-2721/2027.38611

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