A molecular dynamics study on cooling rate effect on atomic structure of solidified silver nanoparticles

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Abstract. The atomic structures and solidification point of silver nanoparticles (SNPs) are studied in a series of molecular dynamics simulations based on the empirical embedded atom methods (EAM). The solidification point is calculated from the extracted potential energy during the cooling process, whereas the atomic structures are analyzed using the common neighbor (CN) method. The results indicate that the structures of the solidified SNPs are very sensitive to both the applied cooling rate and the particle size. We find the critical cooling rate where a glassy structure is observed. Below the critical rate, polycrystalline nanoparticles are formed, where the percentage of the close-packed structures, i.e., FCC and HCP, decreases with increasing cooling rate. Moreover, the proportion of those structures is always larger with a bigger particle size for an identical applied cooling rate. The findings in this study provide useful information for many practical applications where the nanostructure strongly affects thermal management and operational efficiency.

1 Introduction

During the past several decades, research in 3D printing has expanded due to its advantages over a wide range of applications [1,2]. This is because 3D printing is a cost-effective process that allows for the fabrication of complex parts or parts that are not possible to fabricate using other techniques. Silver nanoparticles (SNP), which are not separate from this trend, contribute highly to the 3D printing of conductive complex structures [3]. For example, In 2011, for the first time, 3D printed antennas on curvilinear surfaces were demonstrated using silver nanoparticle inks to create electrically conductive meander lines [4]. In 2013, researchers using 3D printing of cells and SNPs created bionic ears that can “hear” radio frequencies far beyond the range of normal human capability [5]. In 2016, Schneider and his co-workers created a new type of 3D-printed transparent electrodes formed by a grid of gold or silver “nano walls” on a glass surface [6].

In additive manufacturing, micro/nano-scale heat management becomes a key problem, since it greatly affects the thermodynamic properties, as well as the atomic structures of nanoparticles during the heating and cooling processes. However, even advanced experiment methods cannot capture the atomic details of the systems. Computer modelling has become an equal partner with

experiments as joining together descriptions of molecules at close-up and zoomed-out scales [7]. Among many approaches, molecular dynamics (MD) has become a powerful tool in the field of nanotechnology as MD provides physical insight into the understanding at molecular level of processes related to additive manufacturing. E.g. heat transfer across crystal-melt interfaces [8,9] and grain boundaries [10–12], fluid flow past a surface [13–15], melting and crystallization of metallic nanoparticles [16–22].

In a recent MD report, we studied the heating process and found that the thermodynamic properties of SNPs are strongly dependent on the nanoparticle size [16]. This size dependence has also been observed for other metallic nanoparticles such as Cu [19], Au [19], Ni [19,23], Fe [20], etc. Furthermore, the cooling rate has been demonstrated as one of the key factors affecting the structure of nanoparticles during the cooling process and after solidification. For example, Shibuta investigated the solidification of Mo nanoparticles and found that BCC single-crystalline, glassy, and polycrystalline nanoparticles can be formed by manipulating the particle size and cooling rate [17]. In another report, Shibuta and Suzuki revealed that the solidification point of Mo nanoparticles decreases with increasing cooling rate, then drops rapidly at a cooling rate on the order of 10^{12} K/s [18]. Similar investigations on others FCC metals, for example, Ni [19,23], Au [19,24], and Cu [19,25], and several BCC metals [20] have also been conducted. Despite efforts to understand the

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solidification of SNPs [26–28], a general picture is lacking to express the effects of both the cooling rate and the particle size. Furthermore, polycrystalline structures cause grain boundaries (GBs), which greatly affect the thermal transport in nanodevices [10,11]. The introduction of GBs tends to reduce the thermal conductivity of the materials due to thermal boundary resistance. In addition, our recent reports revealed that the atomic structures at the interface play a dominant role in vibrational coupling and energy transfer [8,10]. Therefore, controlling the structure of the 3D/4D-printed nanodevices is critical for thermal management.

For all the reasons given above, we aim to investigate the solidification of SNPs by performing MD simulations. The *objectives* of the present study are to (1) determine the effects of the cooling rate on the solidification point and atomic structure of SNPs containing 2093 atoms (Ag₂₀₉₃), and (2) provide a general picture of the effects of the cooling rate and particle size on the atomic structure of SNPs. Our paper is organized as follows. In Sections 2 and 3, we summarize the computational methods, which include descriptions of the simulation domain and analysis methods of the atomic structure. In Section 4, we present our results and discussion on the effects of the cooling rate and nanoparticle size. Finally, conclusions are presented in Section 5.

2 Computational methods

2.1 Molecular dynamics simulation

All MD simulations are performed using the open-source LAMMPS code [29]. For visualization of the atomistic configurations, we use the free OVITO software [30]. The EAM [31] was applied to model the interatomic forces between atoms. The EAM accurately describes the total energy of a metal by considering the embedding energy as a function of atomic electron density. The total energy E_{total} of system in the EAM potential is represented by

$$E_{\text{total}} = \sum_i F_i(n_i) + \frac{1}{2} \sum_{i,j(j \neq i)} \phi_{ij}(r_{ij}), \quad (1)$$

where ϕ_{ij} is a pairwise potential as a function of the interatomic distance r_{ij} between atom i and atom j , and F is the embedding energy as a function of the atomic electron density $n_i = \sum_{j \neq i} e_j(r_{ij})$, where e_j is the electron density contributed by atom j . By using this EAM potential, in our recent study we found that the melting and solidification points of the bulk silver are in good agreement with experimental values [16].

The SNPs are simulated using the NVT ensemble (i.e., constant particle number, constant volume, and constant temperature) without periodic conditions leading to free cluster surfaces, which follows the method reported by Qi et al. [23]. All clusters are prepared by cutting a spherical region from a large FCC block of Ag. Each cluster is simulated in a large cubic unit cell with a fixed size. We have considered Ag nanoparticles of different sizes ranging

from 225 atoms to 8589 atoms, which correspond to diameters of 2.1 nm–6.9 nm. The simulations were done using a velocity Verlet algorithm to integrate Newton's equations of motion. The simulation time step was set to 1 fs, leading to quite stable dynamic trajectories. The initial velocities of atoms are assigned according to the Maxwell–Boltzmann distribution. All the systems are equilibrated at 300 K for 20 ps before heating. Subsequently, they are subjected to a heat process with a constant and identical rate of $\Delta T/\text{dt} = 1 \text{ K/ps}$ from 300 K to 1500 K. Finally, all the liquid metal droplets are cooled to 300 K at various cooling rates ranging from $2.0 \times 10^{10} \text{ K/s}$ to $2.0 \times 10^{12} \text{ K/s}$.

3 Analysis of atomic structures

The radial distribution function (RDF), $g(r)$, has been widely applied to analyze the atomic structure in amorphous, liquid, and crystalline states, and is given as

$$g(r) = \frac{\langle n_r(r, r + dr) \rangle}{\rho 4\pi r^2 dr}, \quad (2)$$

where ρ is number density given by N/V , with N being the number of atoms in volume V , $\langle n_r(r, r + dr) \rangle$ is the average number of atoms within a spherical shell surrounded by $r + dr$, and $4\pi r^2 dr$ is the volume of that spherical shell.

In order to provide an in-depth analysis on atomic structure, we use the common neighbor (CN) analysis method, which can be thought of as a decomposition of the RDF according to the environment of the pairs [32,33]. The first peak of the RDF describes the nearest neighbors. Defining the first peak to be at $r < r_c$, where r_c is the position of the first minimum of the RDF, and referring to those as “bonded” pairs, each pair of atoms is classified in the following way: a set of three indices, abc (i.e., the local environment of the pair), where the a index is the number of neighbors common to both atoms, the b index is the number of bonds between these common neighbors, and the c index is the number of bonds in the longest continuous chain formed by the b bonds between common neighbors. Next, a radial distribution function for each type of pairs, $g_{abc}(r)$, is obtained once each pair is assigned one of the abc types. These are referred to as the CN components of the RDF and are normalized as

$$g(r) = \sum_{abc} g_{abc}(r). \quad (3)$$

As a result, the total number of pairs corresponding to each peak in the RDF is an efficient measure of the atomic structure. Pairs corresponding to the first peak in the RDF are denoted as $\alpha\text{-}abc$ and their number, $P_{\alpha\text{-}abc}$, is given by

$$P_{\alpha\text{-}abc} = \frac{4\pi N}{V} \int_0^{r_c} r^2 g_{abc}(r) dr. \quad (4)$$

Similarly, pairs corresponding to the second peak, between r_c and the second minimum in the RDF, are denoted as $\beta\text{-}abc$.

Fig. 1. Variations of potential energy per atom with the temperature of Ag_{2093} during the cooling process from 1500 K to 300 K at various cooling rates.

The CN method is an effective filtering method to classify atoms in crystalline systems and is powerful enough to distinguish between various local structures, in particular, FCC, HCP, BCC, and icosahedral environments [33]. Different types of pairs are associated with different types of local order. E.g. (421) bonded pairs of type are the characteristic of FCC and HCP order [30].

4 Results and discussion

We first need to determine the solidification point (T_s) of the nanoparticles. Typically, the solidification point is defined as the temperatures at which the enthalpy changes discontinuously. By thermodynamic definitions, enthalpy changes are related to internal energy changes. Thus, in MD simulations with constant volume conditions, T_s can be determined as the temperature where the potential energy (PE) changes discontinuously due to a difference in atomic ordering (disordered in the liquid phase and crystalline in the solid phase). Therefore, in the present paper, we calculate T_s using the PE data. Figure 1 shows the PE per atom for Ag_{2093} versus temperature at various cooling rates. Typically, there are two linear regimes of PE that are separated by a slow drop or abrupt drop in energy at a certain temperature. For such cases, T_s is approximated as an average temperature value between two temperatures at which the linear decrease in PE disappeared and reappeared. It should be noted that T_s can be additionally defined by either calculating the heat capacity or the Lindemann index as a function of temperature. However, Shibuta demonstrated coinciding T_s values that were obtained from the three different methods mentioned above [17].

For all cases plotted in Figure 1, the PE exhibited similar decreases as temperature decreased to approximately 800 K, irrespective of the cooling rate. However, the PE shows significantly different features below 800 K. The difference in PE per atom with respect to temperature

Fig. 2. Solidification point of Ag_{2093} as a function of the applied cooling rate.

corresponds to the difference in the final structure of the nanoparticles. A discontinuity (i.e. a drop) in the variation of potential energy with temperature in the cooling process implies a polycrystalline nanoparticle is formed at the final stage of 300 K. Meanwhile, glassy structures are formed when the potential energy decreases continuously with temperature (cf. case 2.0×10^{12}). Therefore, we infer that a glassy structure is formed in SNPs by cooling at a rate of 2.0×10^{12} K/s. This is also defined as the critical cooling rate for Ag_{2093} . This is attributed to preservation of the disordered structure in the liquid state during the solidification process from rapid quenching. As a result, the solidification temperature cannot be defined at the critical cooling rate and above. Another reason for this is that the atomic diffusion is restricted at high cooling rates. The obtained critical cooling rate in this work is consistent with other reports [27,28]. However, it is noted that the critical cooling rate is very sensitive to the size of the nanoparticles. Conversely, for a cooling rate of 1.0×10^{12} K/s or less, polycrystalline nanoparticles are generated, indicating the first-order phase transition.

T_s of Ag_{2093} under the different cooling rates studied in this work is shown in Figure 2. The average temperature obtained from five calculations at each condition is plotted. The differences between the T_s values for the cooling rate on the order of 10^{10} K/s are negligible. However, the T_s values significantly decrease when the cooling rates are on the order of 10^{11} K/s. This provides evidence of the effects of the cooling rate on T_s , whereas its effects on the atomic structure of SNPs are presented below.

Next, we start to investigate the effects of the cooling rate on the atomic structure of the nanoparticles. The variation in the atomic structure with different cooling rates can be explained by the RDF and the CN analysis method. Figure 3 shows the RDF analysis results for the final structures of Ag_{2093} at various cooling rates. The series of RDF peaks describes the atomic configurations in the nanoparticles, and thus, it can be concluded that the final structure of the nanoparticles is strongly affected

Fig. 3. RDF of Ag_{2093} at the final stage of the cooling process (i.e., 300 K) under different cooling rates.

by the applied cooling rates as observed for different RDF with different cooling rates. At the critical cooling rate (i.e., 2.0×10^{12} K/s), only the first to third RDF peaks are detectable, confirming that glassy structures are formed with short-range topological ordering. For all cases below the critical cooling rate, the RDF shows a lot of peaks, the positions of which fit the FCC structure. However, only the first three neighbor peaks are exhibited as sharp peaks. These observations imply that the polycrystalline structures in Ag_{2093} are formed at 300 K for the cooling rates investigated here that are less than the critical value. The analysis of RDF also reveals the differences in the formation of polycrystalline structures in these cases. E.g., an applied cooling rate of 6.0×10^{11} or less, the first peak shows more than twelve atoms indicating the significant existence of FCC and HCP structures. This is in contrary for the cases where the cooling rate is greater than 6.0×10^{11} . Therefore, we infer that the lower the cooling rate, the more obvious the crystalline characteristics of the resulting nanoparticles at 300 K.

Figure 4 shows a histogram of the number of atoms of Ag_{2093} with the corresponding cohesive energy at the final stage of the cooling process for the various cases with cooling rates on the order of 10^{10} K/s, 10^{11} K/s, and 10^{12} K/s. The results in Figure 4 are obtained by computing the potential energy of each atom. Subsequently, the histogram is done by selecting all atoms whose potential energy lies within a certain interval. It is found that where the PE shows a peak in the number of atoms is almost the same for all the cases plotted. However, the peak values are different with different cooling rates. This is consistent with the average PE per atom at 300 K, as shown in Figure 1. Here, the results are related to the atomic configuration of the nanoparticles formed after solidification. In other words, the final structure of the SNPs is more stable with a decreased cooling rate.

The atomic structures analyzed by the CN method are presented in Figure 5. Here, we show the results of the

Fig. 4. Histogram of the number of atoms in Ag_{2093} with the corresponding potential energy at 300 K for several cases of cooling rates on the order of 10^{10} K/s, 10^{11} K/s, and 10^{12} K/s.

Fig. 5. Visualization snapshots of Ag_{2093} during the cooling process with various cooling rates. The color of the balls corresponds to the results analyzed by the CN method.

various cases with cooling rates on the order of 10^{10} K/s, 10^{11} K/s, and 10^{12} K/s at the initial stage (i.e., 300 K), at 1500 K after heating, at the solidification point, and at 300 K after solidification. Here, we refer to amorphous structures as the “other” structure. It should be noted that all the surface atoms cannot be detected in their structures because no periodic boundary conditions are applied. In addition, the BCC structure is not found for

Fig. 6. Percentage contribution of various structures at the final stage of the cooling process (i.e., 300 K) of Ag_{2093} obtained from different cooling rates.

any of the cases studied. Without any doubt, the results at the initial stage and at 1500 K are identical. However, the effects of the cooling rate start to appear from the solidification point, and then they are clearly observed at the final stage of the cooling process. From the results in Figure 5, it is evident that the amorphous percentage increases with the cooling rate.

The effects of the cooling rate on the atomic configuration of solidified SNPs are plotted in Figure 6. The percentage of the close-packed structures (i.e., FCC and HCP) reaches $\sim 65\%$ when the cooling rates are on the order of 10^{10} K/s. However, it gradually decreases with increasing cooling rate. At the critical cooling rate, the amorphous structures are observed to occupy $\sim 60\%$. This confirms the preservation of the disordered structure in the liquid state during the solidification process as rapid quenching takes place and atomic diffusion is restricted at such high cooling rates. In 2008, Qi et al. investigated the freezing process of Ag_{429} and revealed that single FCC nanoparticles could be formed at 300 K after enough relaxation, even at the critical cooling rate or below [28]. The interpretation is that the proportion of surface atoms to the total number of atoms is very high for such small nanoparticles, making them unstable. Under such conditions, the nanoparticle may change to more stable configurations according to the thermodynamic law. This is reasonable, as the surface energy is high enough to overcome the energy barrier of the amorphous/polycrystalline-FCC transition for small nanoparticles. However, this phenomenon has not occurred for the cases studied here since the driving force from the surface of the large nanoparticle, i.e., Ag_{2093} , cannot overcome the energy barrier of such transitions.

Our last step is to provide a general picture on the effects of the cooling rate and particle size on the atomic structure of the SNPs. In Figure 7, we show the structure configurations analyzed by the CN method of SNPs containing 225 atoms to 8589 atoms, which correspond

Fig. 7. Visualization snapshots of the atomic structures of the solidified SNPs with different sizes but under an identical cooling rate of 1×10^{12} K/s. The color of the atom balls corresponds to the results analyzed by the CN method. The color of the balls as described in Figure 5 holds for this Figure.

to diameters of 2.1 nm–6.9 nm. All the solidified SNPs in Figure 7 are cooled with an identical cooling rate of 1.0×10^{12} K/s, which is very close to the critical cooling rate. For the smallest SNP studied here (i.e., Ag_{225}), most of the nanoparticle is occupied by amorphous atoms. However, the percentage of the close-packed structures increases with the particle size. For a complete picture, Figure 8 presents the effects of both the cooling rate and particle size on the percentage of FCC and HCP structures formed in the SNPs. The dependence of the atomic structure on the cooling rate is confirmed above. Here, we additionally indicate that the influence of the particle size on the atomic structures are different with different sizes. For instance, at a specific cooling rate, the percentage of closed-packed structures is always larger with a bigger particle. In addition, crystalline structures do not increase monotonically with nanoparticle size, i.e., some fluctuations are observed. This is attributed to the random distribution of grain boundaries in the polycrystalline metal nanoparticles. The fact is that within the uncertainties both Figures 6 and 8 do not show a drastic change in the contribution of each structure that forms the nanoparticle at the final stage. However, the increase of the amorphous structure is still observed. E.g., for the biggest size in this study Ag_{8589} , the amorphous structure increases from 25% to 50% when the cooling rate increase from the order of 10^{10} to 10^{12} . These percentage numbers are from 60% to 88% for the smallest nanoparticle Ag_{225} .

Fig. 8. A general picture of the effects of both the cooling rate and the particle size on the percentage of close-packed structures (i.e., FCC and HCP).

5 Conclusions

In the present study, the EAM potential is applied to investigate the atomic structure of solidified SNPs with various cooling rates and particle sizes using MD simulations. All the SNPs are cooled from 1500 K to 300 K with different cooling rates to extract the PE and calculate T_s . The atomic structures of the SNPs at 300 K are analyzed using the CN method. In addition, we perform the same simulations with different particle sizes to provide a general picture of the effects of both the particle size and cooling rate on the atomic structures of the SNPs. The following results were obtained.

- (i) For Ag_{2093} , the PE of the SNPs shows a similar decrease as the temperature decreased to approximately 800 K regardless of the cooling rate applied. However, significant differences in the PE features below 800 K are observed, which indicates differences in the structures of the solidified SNPs. Furthermore, we find that T_s significantly decreases when the cooling rates are on the order of 10^{11} K/s, whereas the differences between the T_s values for the cooling rate on the order of 10^{10} K/s are negligible.
- (ii) We find a glassy structure when the cooling rate of 1.0×10^{12} K/s is applied, which is in line with other reports. Meanwhile, the polycrystalline structures in Ag_{2093} are formed at 300 K for cooling rates less than the critical value. In addition, the significant existence of close-packed structures (i.e., FCC and HCP) at the final stage of SNPs is observed when the cooling rate is less than 6.0×10^{11} K/s. Importantly, these structures decrease with increasing cooling rate. We also find that the final structure of the SNPs is more stable with decreasing the cooling rate.
- (iii) A general picture of the effects of both the cooling rate and particle size on the nanoparticles is provided. The results indicate that the percentage of

the close-packed structures is always larger with a bigger nanoparticle regardless of the applied cooling rate. Furthermore, the random distribution of grain boundaries in the solidified polycrystalline metal nanoparticles causes a monotonic decrease of the percentage of the crystalline structures with nanoparticle size.

In conclusion, the solidification point and atomic structures of the SNPs are affected by not only the cooling rate, but also the particle size. The findings in this study provide useful information for many practical applications where the nanostructures strongly affect thermal management and operational efficiency.

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Author contribution statement

B.K. designed and supervised the research. T.Q.V. performed the simulations and analyzed data. All authors wrote the manuscript together.

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