

Dominant mechanisms of the sintering of copper nano-powders depending on the crystal misalignment



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ABSTRACT

Sintering mechanisms of nanoscale copper powder are investigated using molecular dynamics (MD) simulations based on the embedded-atom method (EAM). The densification parameters, such as shrinkage, and relative sintered density are calculated using the two-particle sintering model. This paper considers the important role of crystalline misalignment between two particles on densification. Besides volume diffusion contribution, misalignment between the crystal structures results in enhanced grain boundary diffusion. At low temperatures, grain boundary torque cause particles to rotate to reduce grain boundary energy. At higher temperatures, particle rotation becomes complicated including remarkable twist, and grain boundary tilting due to grain-boundary-like diffusion. These results provide insights to the processing cycle parameters applicable to nano-powders.

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1. Introduction

Nanostructured materials draw attention because of the novel physical and mechanical properties compared to bulk materials [1,2]. The Hall-Petch effect, where hardness and strength increase with a smaller crystal grain size, is one example of the potential gain from nanostructured materials. Among processing options for nanostructured materials, sintering of small particles is a cost-effective means to form net-shape components from metal and ceramic powders. One of the most challenging issues in this field is to avoid coarsening during the thermal cycle required to densify the powder; effectively preserving the nanoscale structure while thermally inducing densification. Therefore, it is important to understand underlying sintering mechanisms of nano-powders as the first step to design appropriate methods to control grain growth.

In general, metal powders can sinter by at least five sintering mechanisms: dislocation climb and glide, evaporation-condensation, grain boundary diffusion, surface diffusion, and volume diffusion [3]. Mass flow by volume diffusion involves an exchange between vacancy and atom. Although the vacancy population is on average at equilibrium depending on the temperature, still local vacancy creation or annihilation event at interfaces create a net volume diffusion flow between interfaces. The net effect is a progressive pore filling and densification. Likewise, related events involve atomic motion. If dislocations are present, then atomic transport involves dislocation glide induced by surface stresses or dislocation climb from coupled volume diffusion. If the vapor pressure is sufficient, then transport occurs pores by preferential evaporation from convex surfaces and condensation on concave surfaces. With a high surface area, as is typical to nanoscale particles, surface diffusion is preferred with atomic motion from kinks, ledges, vacancies, or adatom positions decorating curved surfaces. Finally, as bonds form between contacting particles, the misalignment of crystal planes results in a grain boundary in the bond that becomes an active path for grain boundary diffusion and densification. For nanoscale copper powder, the expectation is that during heating surface diffusion, with a lower activation energy and high surface area, will initially dominate

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sinter bonding. As temperature increases, volume diffusion becomes more active, but with the growth of the interparticle bond and its associated grain boundary, then grain boundary diffusion becomes active.

At the nanoscale, the sintering mechanisms involve abnormally rapid bonding and coarsening, not seen with micrometer sizes powders. The specific role of crystal orientation is difficult to ponder at this size scale, unlike the profound experiments of rotating sphere on a plate at the microscale [4–6]. To elucidate sintering mechanisms, molecular dynamics (MD) simulations enable direct consideration of mass transport event in light of specific crystal misorientation. These numerical methods allow direct consideration of crystallographic structure and have been carried out for sintering for various metals such as Cu [7–10], Au [8,9], Pd [11,12], Al [13], Ag [13], and W [14]. Zhu and Averback [7] revealed rapid sintering is due to the high shear stresses in the neck region. This would suggest the initial sintering mechanism is plastic flow. On the other hand, Zeng et al. [8] noticed surface and grain boundary diffusion as the main mechanisms, although dislocations are present at the early stage of the sintering. Raut et al. [13] questioned the importance of both plastic deformation and surface diffusion during the sintering of nano-powders. Other researches generally reported surface diffusion and grain boundary diffusion as the two major sintering mechanisms for metals [15–17].

Meanwhile, several experimental observations have elucidated nano-powders rotate to align themselves along the same orientation to give coalescence [18–20]. Ng and Ngan [19] investigated the real-time coalescence of Ni-Al nano-grains, showing rapid grain rotations to achieve crystallographic alignment for complete grain boundary removal. Jose-Yacamán et al. [20] observed the coalescence of two very small Pd nano-powders using high-resolution TEM (HRTEM). They also showed particle reorientation with a residual grain boundary after coalescence for two 11 nm bimetallic Au-Pd nano-powders, even when atoms rearranged.

In addition, the reorientation of nano-powders is treated by several MD simulations, resulting in the grain boundary energy minimization [8,15,21,22]. Zeng et al. [8] observed fiber rotation for sintering of three fibers with perfect alignment via two-dimensional MD simulations. They thought there might be a driving force to reduce the free surface energy. Ding et al. [22] revealed with two-dimensional problems that a large initial crystalline misorientation leads to the formation of a grain boundary despite reorientation, while small crystalline misorientation leads to grain boundary elimination.

Despite these efforts, the knowledge of sintering mechanisms based on the evolution of crystal structure during sintering of nano-powders is far from comprehensive. Especially, atomic transports in the neck region is not established, especially as related to particle rotation. In present study, sintering mechanisms of nano-powders depending on the crystalline misalignment and the temperature are investigated using MD simulations with the embedded-atom method (EAM). Sintering simulations of two spherical nano-powders are carried out. Subsequently, atomic transports are analyzed using an atom-tracking approach that includes displacement vector of each atom. This approach helps explain the sintering mechanisms. Finally, particle rotation arising during sintering is related to the initial crystalline misalignment.

2. Modeling & simulations

Molecular dynamics (MD) simulations have been carried out using LAMMPS [23,24], which is one of open sources for MD simulations. The embedded-atom method (EAM) approach was employed to describe the motion of atoms. In the EAM approach

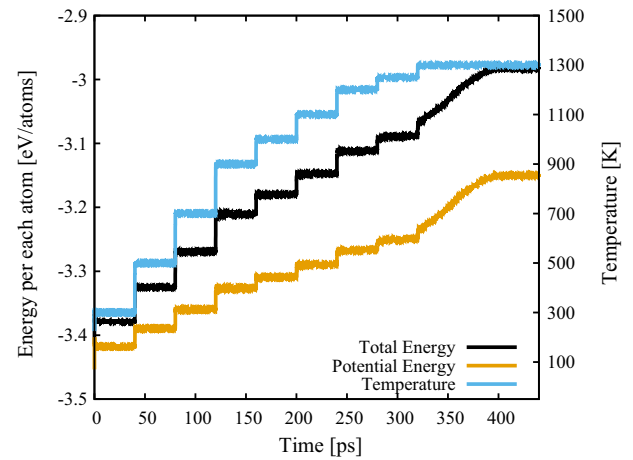


Fig. 1. Evolution of the energy and the temperature during non-isothermal melting. The energy is stable after every 40 ps interval, except for 1300 K. At 1300 K, the energy considerably increases, implying the phase change of a powder.

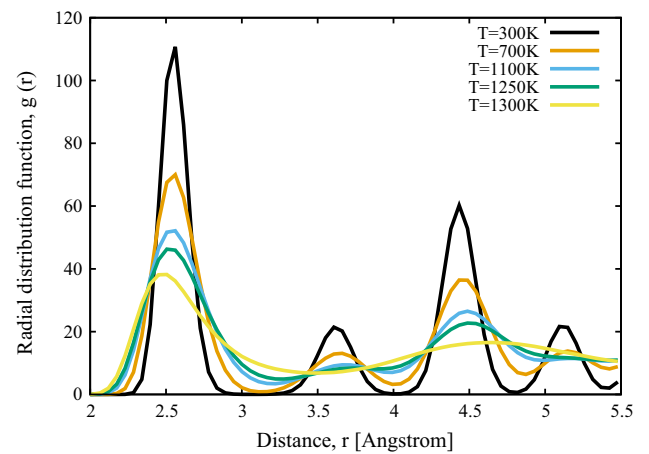


Fig. 2. Radial distribution function with several temperatures. The radial distribution function describes how density varies, which is an indicator to the phase of materials. Below 1300 K, picks are captured clearly, while second pick disappears at 1300 K. The melting point of copper is between 1250 K and 1300 K.

[25,26], total energy E of a system of atoms is written as the sum of the atomic energy,

$$E = \sum_i E_i, \quad (1)$$

with the atomic energy being the sum of two contributions,

$$E_i = \frac{1}{2} \sum_{j \neq i} V(r_{ij}) + F(\rho_i), \quad (2)$$

where $V(r_{ij})$ is an interatomic pairwise potential, and $F(\rho_i)$ is the embedding energy function of the local “atomic density” at the site of atom i . The interatomic pairwise potential represents the interaction between an individual atom and its neighbor as a function of the relative distance r_{ij} . The embedding energy describes the interaction among the electronic orbitals of the atoms. A non-dimensional term ρ_i is also considered to be the contribution of each neighbor atom to the electronic density of a particular atom,

$$\rho_i = \sum_{j \neq i} \rho(r_{ij}). \quad (3)$$

In this paper, EAM parameters of Cu proposed by Mishin et al. [27] were used for the simulations.

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