# Effect of Particle Shape on Nanoparticle Sintering: A Molecular Dynamics Simulation Study


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### Abstract

Sintering of nanoparticles to create films and patterns of functional materials is emerging as a key manufacturing process in applications like flexible electronics, solar cells and thin-film devices. Further, there is the emerging potential to use nanoparticle sintering to perform additive manufacturing as well. While the effect of nanoparticle size on sintering has been well studied, very little attention has been paid to the effect of nanoparticle shape on the evolution of sintering. This thesis uses Molecular dynamics (MD) simulations to determine the influence of particle shape on shrinkage, neck growth, and atomic diffusion for three common nanoparticle shape combinations, i.e., sphere-sphere, sphere-cylinder, and sphere-flake nanoparticles of different sizes. The results from this work show that depending on their relative sizes, both the degree of neck growth and shrinkage are affected by the nanoparticle shape. The possibility of using this phenomenon to control density, neck growth and stresses during nanoparticle sintering are discussed.


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