Investigation of the Formation of Iron Nano-Particles by Molecular Dynamics Simulations

T. Kraska [C, S] and N. Lümmen
Physical Chemistry, University Köln, Köln, Germany

Nano-particles of ferromagnetic metals or alloys are of manifold interest in technical but also medical applications. The special magnetic properties of small systems, such as the increased magnetism compared to the bulk, are reasons for the interest in magnetic nano-particles. The properties of the particles are related to their structure. The structure is the result of the particle formation process which includes nucleation, growth by coagulation or coalescence and sintering. The understanding of the kinetic processes and their dependence on the state conditions makes it possible to steer the process and influence the resulting properties. In this work we investigate the formation of iron particles from the supersaturated vapor phase by molecular dynamics (MD) simulation. The supersaturated metal vapor can be generated, for example, by a decomposition of a precursor gas. In case of simple fluids interacting by van der Waals interactions, an effective pair potential is usually employed. In case of metals, many-body interactions have to be accounted for. The formation of iron particles from the gas phase is investigated at different state conditions. One can recognize differences in the structure as well as in the roughness or the difference in the surface/volume ratio.