

Surface Phenomena and Phase Change in Nanoparticles and Nanodroplets

Salvatore Arcidiacono and Dimos Poulikakos

Laboratory of Thermodynamics LTNT, Institute of Energy Technology,
ETH Zurich, Sonneggstrasse 3, CH-8092 Zürich,

Surface phenomena are very important in nanoscale systems and technologies because they exhibit a very large surface to volume ratio.

Molecular dynamics (MD) simulations are used here to investigate such phenomena where the continuum approach breaks down. The study is focused on nanodroplets and nanoparticles.

The thermodynamic parameters of an argon nanodroplet such as surface tension, density and pressure profiles are calculated for three different temperatures and compared with the corresponding experimental values. The interface thickness of the droplet is characterized by an intrinsic contribution and a contribution due to capillary waves and is evaluated both numerically and analytically. The free oscillations of the above mentioned nanodroplets and the limit of the applicability of continuum theory for such oscillations are also studied. Although the simulated system cannot be considered strictly as a continuum, a good overall agreement is found.

The melting and the coalescence process of two gold nanoparticles for a host of initial temperatures and starting radii (from 9.5 to 25 Angstroms) in vacuum are studied. The findings of MD simulations for particle melting are in well agreement with experiments. Diverse mechanisms of the first sintering stage, characterized by a growing neck region, are found. The results are also compared with a phenomenological macroscopic model based on an energy balance and supplemented by a model for the surface variation of the nanosystem under consideration. Accounting for the findings of the MD simulations for the neck growth rate, the validity of the analytical model with the initial temperature and radius of the particle is shown.