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Author Jun-Wei Chiu
Author's Email Address No Public.
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Abstract
In this study, the thermal stability, structural properties, and coalescent characteristics of copper and ZnO nanoparticles under different temperatures are explored by molecular dynamics and experiments. In the canonical ensemble, Tight-binding potentials were used to simulate characteristics of the nanoparticles. To understand the thermal critical temperatures and the structural properties of the nanoparticles, the mean-square-displacement curves and radial distribution functions were carried out after a constant increasing heating process. In experimental parts, atomic force microscope (AFM), energy dispersive spectrometer (EDS), optical microscope (OM) and scanning electron microscope (SEM) were employed to measure the microstructures of the nanoparticles. The experimental results were compared with those of molecular dynamics simulations. Results showed that the melting temperatures of the nanoparticles decreased as the diameter of the nanocluster decreased. In the aggregations of different number nanoclusters, the shrinking rate increased when the heating temperatures increased, but it decreased as the numbers nanoclusters decreased. The absorbing and spreading behaviors of the nanoparticles on the substrate surface were changed due to different sizes of the nanoparticles and the interfaces between the nanoparticles and the substrates. Furthermore, this study provides the thermal characteristics of nanoparticles on substrate surfaces or free standing states to improve the applications of nanoparticles in the fields of nanotechnology.
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