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Structural properties and thermal stability of Ni-Cu and Ni-Al core-shell spherical nanoparticles

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Understanding of thermodynamic behaviors and stability of bimetallic core-shell nanoparticles (CSNPs) is of significance for their wide range of applications such as catalysis, optic, biomedicine, and energy storage. Here we systematically investigate thermodynamic and structural properties of Ni@Cu, Cu@Ni, Ni@Al and Al@Ni core-shell nanoparticles by using molecular dynamics simulations with embedded atom model (EAM). The spherical CSNPs model system with diameter close to 6 nm were prepared with different shell thickness. The heating and fusion process was analyzed by calculating the potential energy, radial distribution function, Lindemann index and polyhedral template matching tool. In addition, to analyze the thermal stability of the CSNPs, the annealing process is carried out at different temperatures and the mean square displacement is calculated as well as the diffusion coefficient for each component. The results of the simulation show that unlike the case of Cu-Ni, where the typical behavior of the heating curve is observed, in the Ni-Al system the potential energy with temperature presents a peculiar behavior that depends on the relationship of the thickness of the layers as well as the rate of heating. The analyzed CSNPs keep their core-shell arrangement up to annealing temperatures of the order of 800K

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