Computer Simulations of Interactions Between Hematite Nanoparticles

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The study of hematite nanoparticles has been proposed to evaluate the interaction and coalescence in polydisperse systems, in which larger nanoparticles growth at expense of the smaller ones have been observed experimentally. For this purpose, different slab models with facets {104}, {110} and {100} have been used to simulate a large nanoparticle surface meanwhile a small two nanometers sphere has been used as a model for the small nanoparticle. Our simulations were performed by molecular dynamics simulations using classical force fields. In order to evaluate the behavior of the system as a function of the temperature, the systems were heated from 300 K to 1200 K. After theses processes, the systems were cooled down to 300 K again. In addition, equilibrium simulations have been made at constant temperatures (300 K, 400 K, …, 1200 K). The analysis of density after heating and cooling have shown similar patterns for both slabs and spheres. For all facets studied the radial distribution of function for Fe (slab) – O (sphere) have shown that the peaks are more structured at 900 K compared with 800 K because at higher temperature the atoms of the sphere have enough energy to reorganize and align its planes in response to the exposed crystallographic facet by a atomic diffusion process. Hence, the transition temperature, minimum temperature where the spheres restructure in the crystallographic direction of the slabs, was found between 800 K and 900 K for all facets studied. !

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