Nanoscale physics

Molecular dynamics simulations of the oxidation of zinc nanoclusters

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We carried out molecular dynamics simulations of the oxidation of zinc nanoclusters to investigate the process of the formation of Zn-ZnO core-shell nanostructures. This structure is promising material as a working environment in gas sensors [1]. We performed simulations with three initial temperatures, three different initial oxygen density and two initial sizes of Zn nanoparticles. Depending on this it is possible to obtain different by structure, oxide layer thickness and shape Zn-ZnO core-shell nanoparticles.

The study of structural and electronic properties of small ZnO nanoparticles conducted in works [2, 3]. In the present work it is shown that the structure, shape and oxide layer thickness of the obtained particles directly depends on the initial oxygen density and initial temperature of the system. At increasing of initial oxygen density the oxide layer thickness of obtained nanoparticles increase to a certain limit. During the analysis it was found, that created clusters mainly preserved their structure of core, but structure of shell commonly was amorphous. The results are in good agreement with experimental results and earlier molecular dynamics simulations.

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