Nanoscale physics

Molecular dynamics study of the condensation of zinc oxide from the gas phase

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We carried out molecular dynamics simulations to investigate the process of formation of ZnO nanoclusters from the gas phase. To describe the interaction between atoms we used the reactive force field [1]. We have been studied the influence of cooling rate and concentration of atoms on the physical parameters of obtained nanoparticles. Six computer experiments was conducted with different initial cooling rates and concentrations. Depending on this it is possible different mechanisms of cluster growth.

The study of structural and electronic properties of small ZnO nanoclusters conducted in works [2, 3]. In the present work it is shown that the processes of condensation of atoms from the high-temperature gas environment are divided into several stages: nucleation, coalescence and agglomeration, aggregation and coagulation. It is shown that the structure, shape and size of the obtained particles directly depends on the cooling rate of the system. At reduction of cooling rate the number of obtained nanoparticles decreases and their size increases. During the analysis it was found, that created clusters mainly are formed in three structural phases - amorphous, hexagonal wurtzite and cubic zincblende.

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