Study of the threshold crystallization rate of Si–Al and Si–Au nanoparticles with molecular dynamics method

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In connection with the development of the laser printing methods, it is important to study the structure of silicon nanoparticles with impurities of gold and aluminum, since such objects demonstrate various practically important optical and electromagnetic properties depending on the structure obtained upon cooling [1]. In this work, a study of the crystallization of three-dimensional particles was carried out. The method consists in cooling the melt to room temperature. Next, the structure of the nanoparticles was analyzed and the threshold cooling rate required for crystallization was calculated [2]. A wide range of metal impurity concentrations was considered. There are presented the values of the threshold velocities for nanoparticles with a radius of 20 nm. The data obtained are consistent with the images obtained during the experiment for Si–Au nanoparticles. The results of the work are aimed at predicting the physical properties of nanoobjects of a similar structure. All calculations were carried out using a new potential (developed for the LAMMPS package [3]), which was created in the last year, which correctly describes such systems [4].

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