Study of crystallization processes of Si-Al and Si-Au nanoparticles with molecular dynamics method

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Silicon nanoparticles with impurities of gold and aluminum demonstrate different properties which are important in creation of biosensors, high-speed data processing, maintenance of fluorescence, nonlinear optics. All physical features of nanoparticles are dictated by crystal structure [1].
In this work, a study of the crystallization of three-dimensional melted particles was carried out. In result objects with a complex granular structure were obtained. the threshold cooling rate required for crystallization was calculated [2] in a wide range of concentration of impurity metals.
The data obtained are consistent with the images obtained during the experiment for Si-Au nanoparticles. The results of the work will allow to design the real physical objects with properties set ahead. All calculations were carried out using a new potential (developed for the LAMMPS package [3]), which was created in the 2020, which correctly describes such systems [4].

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[2] Makarov S et a 2018 *Nanoscale* **10** 11403–11409
[3] Plimpton S J 1995 *Journal of Computational Physics* **117** 1–19
[4] Starikov S et a 2020 *Computational Materials Science* **184** 109891