Molecular dynamics simulation of lead melt with iron and oxygen admixtures

Khnkoian G V[1,@], Nikolaev V S[1,2] and Stegailov V V[1,2]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[@] khnkoian.gv@phystech.edu

Liquid lead is a promising coolant for the first cooling circuit of a nuclear reactor. Due to the operating conditions, the lead melt contains impurities, including iron and oxygen. Atom binding, growth of solid particles, and the consistence of the solution are of the practical interest.

In the current work, a melt of lead with iron and oxygen admixtures evolution is considered. Modeling is performed by classical molecular dynamics methods using the LAMMPS software package. In the course of the work, the formation of clusters from atoms of iron and oxygen is calculated, the solvation shell of oxygen in lead is analyzed as necessary condition for model credibility.

It is shown that the temperature of the melt and the concentration of the components have an effect on the formation kinetics of clusters from iron and oxygen. The composition of the clusters in the melt at different temperatures and the values of the diffusion coefficients for oxygen and iron in lead are obtained.