Formation of Pb–O in a disturbed flow of liquid lead: A molecular dynamic approach

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Today, the oxygen behavior in heavy liquid metal coolant (HLMC) is studied from the two theoretical perspectives. The first is based on the thermodynamic considerations that allow to derive the appropriate range of the oxygen concentration [1] and to describe nucleation with the models based on the classical nucleation theory [2]. However, these models require insights into microscopic processes. The second is the *ab initio* atomistic approach. It reveals the chemical state of impurities [3], but only allows the study of a few impurity atoms. Molecular dynamics (MD) calculations using empirical interatomic potentials can provide a link between the two mentioned methods. Two interatomic potentials are developed for the system of lead melt with dissolved oxygen. These models accurately reproduce the transport properties of the atoms and also the temperature dependence of the oxygen solubility limit in molten lead. Using the developed potentials and the approach to study disturbed flow in the MD calculation [4], we obtain the pre-turbulent mode of the flow for molten lead. The first attempt is made to calculate the spectrum of the passive scalar (oxygen) in the molten lead flow.

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