Interatomic potential for a system of liquid lead with dissolved oxygen

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Liquid lead is a promising coolant for the first cooling circuit of the next generation fast reactors. Due to the operating conditions, the lead melt contains impurities, including oxygen. The effect of oxygen concentration on the physico-chemical state of dissolved oxygen in liquid lead is still an open issue [1]. Also, accurate calculations of nucleation and dissolution kinetics for solid lead oxide particles in liquid lead are of practical interest.

For further studies of oxygen behavior in liquid lead on the atomic level, we introduce the classical interatomic potential for the system of liquid lead with dissolved oxygen. First-principle calculations are conducted in the VASP software to create the training database. The obtained potential is verified by comparison with ab-initio data and validated on the available experimental data [2] for the conditions typical for the reactor systems.

The agreement between the suggested model and ab-initio and experimental values is demonstrated. The potential reproduces the radial distribution functions obtained in the ab-initio calculations. Melting temperatures and oxygen solubility in liquid lead are in accordance with experimental values. We also qualitatively describe oxygen behavior at different concentrations in lead.

[1] Gladinez K, Rosseel K, Lim J, Marino A, Heynderickx G and Aerts A 2017 *Physical Chemistry Chemical Physics* **19** 27593–27602

[2] Gromov B and Shmatko B 1996 *Izvestiya Vysshikh Uchebnykh Zavedenij. Yadernaya Ehnergetika* 35–41