Solid-liquid interfacial energy in two-component metallic systems – molecular dynamic study

Vadim V. Korolev[1], Vladimir M. Samsonov[2], Pavel V. Protsenko[1]

[1]*Lomonosov Moscow State University, Chemistry Department, Leninskie Gori, 1, str.3, Moscow, 119991, Russia*

[2]*Tver State University, Zhelyabova ul., 33, Tver, 170100, Russia*

korolev@colloid.chem.msu.ru

The solid-liquid interfacial energy characterizes the interaction intensity of adjoining phases and makes it possible to estimate strength reduction and corrosion resistance in the presence of active liquid component. Experimental measurement of interfacial energy for metallic systems is associated with considerable difficulties, therefore molecular dynamic simulation could be considered as an alternative way.

In this study, we have proposed for a first time a method for the interfacial energy calculation in two-component systems based on classical nucleation theory, namely on the Gibbs-Freindlich-Ostwald equation. The essence of this method deals with determination of critical size of spherical nucleus. Earlier, the simulation of nucleation for the determination of interfacial energy was carried out only for one-component systems [1].

The simulations were carried out for the copper/lead solid-liquid system. Simulation was performed using freely distributed LAMMPS in 1025 – 1100 K temperature range. EAM interatomic potential, developed in [2], was used for Pb-Cu couple. To determine the critical size of the nucleus, two parameters were varied: the initial size of the spherical nucleus and the supersaturation. Components activities were estimated under the regular solution assumption.

The obtained values of the interfacial energy are close to those obtained for one-component solid Cu - liquid Cu system, which could be related to the absence of surface activity of lead on the solid/liquid interface. This is consistent with the experimental data obtained for the Pb/Cu system by the multiphase equilibrium method [3].

During the growth of the crystalline nucleus, the formation of lattice defects (grain boundaries) was revealed. This observation can be explained by the high rate of nucleation process.

References:

[1] Huaguang Zhou, Xin Lin, Meng Wang, Weidong Huang, J. Cryst. Growth **377**, 107 (2013).

[2] Jeffrey J. Hoyt, Justin W. Garvin, Edmund B. Webb III, Mark Asta, Model. Simul. Mater. Sci. Eng. **11**, 287 (2003).

[3] Vadim A. Timoshenko, Vladimir Yu. Traskine, Sergey N. Zhevnenko, Pavel V. Protsenko, J. Phys. Chem. C **120** (2016).