Molecular dynamics simulation of Al-Cu alloys

P. Yakibchuk[a], V. Patsahan[a], T. Patsahan[b]

[a] *Department of Metal Physics, Ivan Franko National University of Lviv, 8 Kyryla Mefodiya Str., 79005 Lviv, Ukraine, E–mail: pavioros@gmail.com*

[b] *Institute for Condensed Matter Physics, 1 Svientsitskii Str., 79011 Lviv, E–mail: tarpa@icmp*

The Al-Cu alloys are widely used in a light material production. Their practical application is dictated by distinctive characteristics such as a low density, a high melting temperature and a good thermal conductivity. In literature, one can find a variety of experimental data related to these alloys, while there is a lack of computer simulation studies, which could expand our knowledge about microscopic behavior in the given melts. In our study the method of molecular dynamics is applied to calculate the structural and dynamic properties of Al-Cu alloys. One of the main peculiarities of the classical molecular dynamics is a choice of model potentials of interionic interaction, especially when metal systems are under consideration. In our previous studies we have realized that it is not possible to get sufficiently accurate results with effective pair interionic potentials. Therefore, we used the embedded atom method (EAM) based on the potential, which consists a many-body contribution to the interaction taking into account electron density distribution. On the other hand the EAM can be easily combined with the molecular dynamics method and it is proved to give highly reliable results for a number of pure liquid metals and some alloys. We considered different compositions of the Al-Cu alloys and for each case of them the melting temperatures is obtained. The radial distribution functions and diffusion coefficients for the Al-Cu melts near the melting points are obtained. Also the viscosity and thermal conductivity depending on temperature are derived using the method of non-equilibrium molecular dynamics. The obtained results show a good agreement with experimental data.