Interaction of carbon nanoparticles with liquid and crystalline aluminum

Reshetniak O B[1,@], Reshetniak V V[1,2], Aborkin A V[2] and Filippov A V[3,1]

[1] State Research Center of the Russian Federation—Troitsk Institute for Innovation and Fusion Research, Pushkovykh Street 12, Troitsk, Moscow 108840, Russia

[2] Vladimir State University, Gor'kogo 87, Vladimir 600000, Russia

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

[@] viktor.reshetnyak84@gmail.com

The fabrication and study of the properties of aluminum-matrix composites filled with carbon nanoparticles is of considerable interest [1]. The key issues here are the ensuring adhesion between the matrix and the filler and the uniform distribution of nanoparticles in the matrix material. These issues are largely determined by processes at the interfaces between the matrix and the filler, for the study of which the atomistic modeling is appropriate.

In this work, we propose an atomistic study of the interphase interaction between aluminum and carbon nanoparticles of various morphologies: graphite, graphene, carbon nanotubes, and fullerene-like particles of various diameters. The results were compared with experiments [2, 3]. It is shown that the interaction between Al and C atoms depends on the curvature of the nanoparticle surface, and it is well described by the Lennard-Jones potential. The parameters of the potential are linearly dependent on the average particle curvature. Capillary effects at the interface and coagulation of nanoparticles in an aluminum melt are studied using the example of C_{60} fullerenes. It was found that coagulation is significantly slowed down by the interaction of a capillary nature between fullerenes.

[1] Hu Y, Shenderova O A, Hu Z, Padgett C W and Brenner D W 2006 *Reports on Progress in Physics* **69** 1847

[2] Oh S I, Lim J Y, Kim Y C, Yoon J, Kim G H, Lee J, Sung Y M and Han J H 2012 *Journal of alloys and compounds* **542** 111–117

[3] Hamza A V, Dykes J, Mosley W D, Dinh L and Balooch M 1994 *Surface science* **318** 368–378