Model of structural phase transitions in Al–Cu alloys

Grachyova N A[@], Fomin E V and Mayer A E

Chelyabinsk State University, Bratiev Kashirinykh Street 129, Chelyabinsk 454001, Russia

[@] nagra45da@gmail.com

Molecular dynamics (MD) simulations using the LAMMPS software package and the ADP potential of Al–Cu solid solution compression showed the nucleation and movement of dislocations as well as the phase transition of the crystal structure. Based on the MD simulation results, we formulate a stress relaxation model taking into account the plasticity process and evolution of the phase structure. A feed-forward artificial neural network is used as the equation of state, which takes into account the proportion of copper in the alloy as a continuous variable. The Bayesian parameter identification method is used to determine the coefficients of models of phase composition evolution and dislocation plasticity of metals.

The study was funded by a grant from the Russian Science Foundation (project No. 20-11-20153-P, https://rscf.ru/en/project/23-11-45024/).