Interaction of the edge dislocation with clusters of copper atoms in the aluminum crystal

Fomin E $V^{@}$ and Krasnikov V S

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

[@] fomin33312@gmail.com

Investigation of metal alloys represent is a very relevant problem, because they are widely used for practical tasks. Solid solutions are of particular interest [1]. As shown in the previous work, the interaction of the edge dislocation with copper atoms in the aluminum solid solution can be represented as the interaction of dislocation with individual groups of copper atoms [2]. In this work, we consider the interaction between the edge dislocation and the cluster of copper atoms with various concentrations (20%, 50%, 80% and 100%) in the aluminum crystal. The aluminum single crystal has a size of 52x60x15 nm and crystallographic directions $[\overline{1}10][111][11\overline{2}]$. The edge dislocation is created by inserting an atomic half-plane into the aluminum crystal, and the cluster of copper atoms with a size of 1 nm is created by substituted aluminum atoms in the dislocation path. The dislocation moves in the process of shear deformation, which is performed by the molecular dynamics method [3], where the interatomic interaction is described by the EAM potential [4]. The continuous model of this interaction process is proposed on the basis of previous works that study the interaction of the edge dislocation with structured inclusions [5].

- Varvennea C, Leyson G, Ghazisaeidi M and Curtin W 2017 Acta. Mater. 124 660–683
- [2] Fomin E and Krasnikov V 2020 JPCS 1556 012050
- [3] Plimpton S 1995 J. Comput. Phys. 117 1-19
- [4] Apostol F and Mishin Y 2011 Phys. Rev. B 83 054116
- [5] Krasnikov V and Mayer A 2019 Int. J. Plast. 119 21-42