Motion of Dislocation in Aluminum with Various Copper Strengthening Phases: MD Simulations and Continuum Modeling

Vasiliy S. Krasnikov*, Alexander E. Mayer†, Viktor V. Pogorelko††, Evgeniy V. Fomin†††, Dmitriy S. Voronin††††

Chelyabinsk State University, Bratiev Kashirinykh 129, 454001, Chelyabinsk, Russia
*e-mail: vas.krasnikov@gmail.com, †mayer@csu.ru, ††vik_ko83@mail.ru, †††fomin33312@gmail.com, ††††v-demonizerus@mail.ru

ABSTRACT

We use MD calculations for studying of dislocation slip in aluminum containing strengthening phases of copper in form of solid solution, GP (I, II) zones, teta’, teta’, teta phases. The behavior of edge dislocations in aluminium with precipitates is investigated. In the most considered cases, the dislocation line passes through the obstacle; and only the smallest obstacles are overcome by dislocation bypass. It is shown that first events of overcoming of large obstacle occur due to formation of defect area in aluminum matrix around the strengthening inclusion; the third or fourth ones typically lead to shearing of obstacle, even in the case of such hard inclusion as teta’ phase; and only GP I zones are sheared after the first interaction with dislocation.

We find the dependencies of overcoming stress for dislocation on distance between and on radius of precipitations. The temperature dependence of critical stress is investigated for fixed distance and radius of inclusions.

We offer simple mechanical model of overcoming obstacle by dislocation with only one fitted parameter, which is energy of dislocation per unit of length. The equations are formulated in assumption of constant properties of inclusions during interactions with dislocation. It is necessary to include the dependence of dislocation energy on temperature to obtain the agreement of the modeled data with the MD calculations.

The work is supported by the Russian Science Foundation, grant No. 18-71-10038.