Effect of hydrogen atoms on the deformation behavior of Al-Cu alloy

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In this work, the effect of hydrogen atoms accumulated on θ' phases on the deformation behavior of Al-Cu alloy during shear and tension is studied by the molecular dynamics. The effect of size, temperature, and rate on deformation development in the considered systems is studied. In the work we considered systems containing inclusions of two types of θ'. The first type of systems contains cylindrical inclusions θ' with diameters of 5 and 10 nm, which correspond to the maximum aging strength. The second type of systems is a parallelepiped, one half of which is the θ' layer, and other is aluminum layer, which makes it possible to consider the large θ' layers observed in overaged alloy. It is shown that for all the considered systems, the shear stresses in the systems decrease with accumulation of hydrogen atoms. For systems with cylindrical inclusions, the softening of the θ' phase is observed during precipitate-dislocation interaction in the presence of hydrogen atoms. It is shown that an increase in the number of hydrogen atoms leads to the change of the dislocation-precipitate interaction mechanism. The formation of the Orowan loop, which occurs in the absence of hydrogen, is replaced by the cutting of precipitates. When hydrogen is added to the system, dislocations will nucleate at a lower strain. We observed generation dislocation from the interface in the systems with hydrogen and in the aluminum layer for systems without hydrogen. The dislocation-precipitate interactions was studied using the LAMMPS. The interaction of atoms is described by the BOB potential [1]. The analysis and visualization of the obtained atomic distributions is carried out using the OVITO.

This work is supported by the Russian Science Foundation, Agreement No. 18-71-10038-P.

[1] Zhou X W, Wardb D K and Fosterc M E 2018 *New J. Chem.* **42** 5215–5228