Precipitate strengthening of Al-Cu alloys: A multiscale dislocation dynamics approach

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ABSTRACT

Precipitation hardening is one of the most efficient strategies to increase the yield strength of metallic alloys. Continuum models, based on the Orowan mechanism, have been developed to analyze the potential of the precipitate size, shape, orientation and spatial distribution on the improvement on the critical resolved shear stress on the different slip systems. Although these models were able to rationalize some the experimental trends, it should be noticed that the Orowan model assumes a very simplistic approach for the dislocation/precipitate interaction: the precipitates are rigid obstacles overcome by the formation of an Orowan loop.

In this investigation, the strengthening provided by two types of precipitates (either Guinier-Preston zones or θ'') in an Al-Cu alloy are studied by means of 3D dislocation dynamics [1]. The precipitates have a disk-shape with the broad faces parallel to the (100) planes of the FCC Al lattice and the details of the dislocation/precipitate interaction at the atomic level are analyzed by means of molecular statics and molecular dynamics simulations. The information obtained from the atomistic simulations (whether the precipitates are sheared or by-passed by dislocations, dislocation mobility, etc.) are used as input for the 3D dislocation dynamics analysis so, in so far it is possible, the parameters of the dislocation dynamics simulations are not arbitrary but provided by simulations at lower length scales.

The 3D dislocation dynamics results, together with the corresponding atomistic simulations, were used to ascertain the effect of different parameters (precipitate type, size and volume fraction, dislocation/precipitate orientation, off-set from the dislocation glide plane, dislocation character, etc.) on the actual deformation mechanisms (either precipitate shearing or looping, cross-slip, etc.) and on the strengthening provided in each case.

REFERENCES

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