Precipitate strengthening in Mg alloys: atomistic simulations and experimental observations

G. Esteban-Manzanares*, I. Papadimitriou*, R. Alizadeh†, A. Ma*, J. LLorca*†

*IMDEA Materials Institute. C/Eric Kandel 2, 28040 – Madrid, Spain
http://www.materials.imdea.org

†Department of Materials Science. Polytechnic University of Madrid, 28040 -Madrid, Spain
http://www.materiales.upm.es/dcm/

ABSTRACT

Plastic deformation of Mg and Mg alloys takes place by dislocation glide in three different slip systems (basal, prismatic and pyramidal slip) as well as by tension twinning. Basal slip is the softest slip system in Mg, and increasing the critical resolved shear stress for dislocation slip in this system is necessary to improve the yield strength of Mg alloys and to reduce the plastic anisotropy. Dispersion of nm-sized intermetallic precipitates is the most effective strategy to increase the flow strength of most metallic alloys but this mechanism is not very effective in Mg alloys.

Precipitate strengthening in Mg-Zn was studied by means of micropillar compression tests at different temperatures. The mechanisms of dislocation/precipitate interaction were analysed through transmission electron microscopy of the deformed micropillars. Basal dislocations were able to shear the precipitates but evidence of dislocations bowing between the precipitates was also found. In addition, the critical resolved shear stress decreased with temperature.

In order to understanding these results, atomistic simulations of the dislocation/precipitate interactions were carried out in Mg-Al and Mg-Zn alloys using a new interatomic potential. The matrix/precipitates interfaces are semi-coherent or incoherent in these systems, and a new strategy was developed to identify and introduce in the atomistic model the interfaces with minimum energy. Molecular statics and dynamics simulations of the dislocation precipitate interaction showed similar mechanisms. The first basal dislocation was attracted by the precipitate/matrix interface, propagated along the interface and finally entered the precipitate but was not able progress further because of the large resistance of the precipitate to be sheared. Thus, the dislocation bypassed the precipitate by the formation of an Orowan loop, that remained within the precipitate near the interface. This dislocation loop was not able to progress further until more dislocations bypassed the precipitate and pushed the initial loop to shear the precipitate. This process was eventually repeated as more dislocations overcome the precipitate and these mechanisms were in good agreement with the experimental results. Shearing of the precipitates by basal dislocations in Mg alloys is favoured because the Mg basal plane (which is the most closely packed) was parallel to one crystallographic planes of the precipitate which tend to grow parallel to the basal plane. These crystallographic orientations correspond to (0001)\text{Mg}||\langle 2\bar{1}10\rangle_{\text{p}} in Mg-Zn and to (0001)\text{Mg}||\langle 110\rangle_{\text{Mg}_{17}\text{Al}_{12}} in Mg-Al alloys.

The results of the molecular dynamics and statics simulations were used to determine the influence of precipitate size and spacing as well as the temperature on the critical resolved shear stress to overcome the precipitates by basal dislocations.