MODELING DYNAMIC STRAIN AGING OF ALUMINUM-MAGNESIUM ALLOYS

By

Dawei Zhang

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Approved by the
Examining Committee:

Catalin R. Picu, Thesis Adviser

Frédéric Barlat, Member

Jacob Fish, Member

Hanchen Huang, Member

Antoinette M. Maniatty, Member

Rensselaer Polytechnic Institute
Troy, New York

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ABSTRACT

Jerky flow or the Portevin-Le Chatelier (PLC) effect is observed in dilute alloys in certain conditions. It results from the dynamic interaction of mobile dislocations and solute atoms. Solute atoms diffuse to and age mobile dislocations while they are temporarily arrested at obstacles on their slip plane, which is referred to as dynamic strain aging (DSA). This thesis presents atomistic studies and continuum modeling of solute clustering and solute diffusion in Al-Mg alloys, which are considered elements of the mechanism of dynamic strain aging.

Solute clustering in Al-Mg binary alloys is studied by means of Monte-Carlo simulations. The clustering of Mg is analyzed in the undistorted Al lattice, as well as in presence of dislocations. In the undistorted lattice, Mg has a tendency to form a coherent phase. The binding energy of this structure is rather low and it dissolves at room temperature when only dynamic associations of doublets or triples of solute atoms are observed. Applying a homogeneous hydrostatic strain has no effect on clustering. In presence of dislocations and at room temperature, Mg clusters at cores forming the coherent phase observed in the undistorted lattice at lower temperatures. Clustering at the cores of all types of dislocations is investigated. It is shown that the size, shape and structure of the cluster cannot be predicted by elementary calculations based on the pressure field generated by the unclustered dislocation. Furthermore, the field of the clustered dislocation is compared with that of the unclustered defect.

Diffusion for Mg in Al-Mg alloys is investigated by Molecular Statics and the Nudged Elastic Band method. The activation energy for diffusion of Mg in the bulk is evaluated in the dilute solution limit for the nearest neighbor and the ring mechanisms. It is concluded that bulk diffusion at low and moderate temperatures must be assisted by vacancies. Further, diffusion of Mg along the core of edge, 60° and screw dislocations is studied. The vacancy formation energy in the core and the migration energy for vacancy-assisted Mg is evaluated for a large number of diffusion paths in the core region. It is observed that, similar to the bulk, Mg

diffusion in absence of vacancies is energetically prohibitive. The paths of minimum activation energy are identified for vacancy-assisted diffusion, for all three types of dislocations. The lowest energy path is found in the core of the 60° dislocation, its activation energy being 60% of the activation energy in the bulk. Most diffusion paths have the activation energies larger than 75% of the equivalent bulk quantitiy. This analysis shows that pipe diffusion, which is currently considered as the leading mechanism responsible for dynamic strain aging in these alloys, is too slow in absence of excess vacancies.

The time-dependent Mg solute clustering process is studied using a continuum model calibrated based on atomistic information. The solute atmosphere around an edge dislocation is evaluated in terms of a chemical potential gradient, which is obtained from Monte-Carlo simulations. The solute clustering process is modeled by coupled diffusion-deformation partial differential equations (PDEs). The PDEs are implemented with a plane strain formulation and numerically solved with ABAQUS general purpose finite element program. The evolutions of cluster size and concentration at various selected sites are investigated. The calculation results are compared with Louat's model and atomistic simulation results.

These studies provide a number of important insights into the physics of DSA, as follows: diffusion in the core region and along the pipe has to be assisted by vacancies; this process has a dynamics that may be described by Louat's equation provided the monitored quantity is a specific measure of the cluster size discussed here; cluster growth by bulk diffusion at room temperature is very slow; if cluster saturation is reached, the precipitation of Al_3Mg phase is observed at dislocation core; at constant chemical potential, the solute concentration depends on the hydrostatic component of the strain and not on its deviatoric component.