Micromechanical modelling and atomistic simulations of solute atom segregation towards grain boundaries in Mg

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Abstract

Alloying has been proven to have broad potential for enhancing the poor ductility of magnesium alloys which is associated to an insufficient number of easy slip systems and the development of twinning. Segregation behaviour of solute atoms at grain boundaries (GB) has been widely reported to affect GB stability, GB migration, and crystallographic texture of Mg alloys. It is therefore important to gain a deeper fundamental understanding of the origin of the GB segregation phenomena for the tailored properties material design of Mg alloys. A solute atom can be represented by a point force distribution, corresponding to the forces imposed on the surrounding atoms. The first order moment of this distribution, named *elastic dipole*, can be used to evaluate the long-range elastic fields due to the presence of the solute. Using the method described in (1), the permanent elastic dipole, which can be related to a size and a shape effect, and the polarizability tensor, which is related to the change of the elastic moduli, have been determined by atomistic simulations considering an Y atom embedded in a Mg matrix. Then, the interaction energy between the elastic dipole and the stress fields of several symmetric tilt grain boundaries have been calculated, with tilt axis along and directions. The stress fields have been evaluated from the Virial stress fields provided by molecular static simulations or from the stress fields of dislocation walls, either in heterogeneous anisotropic elasticity using Stroh's formalism (2), or in isotropic elasticity considering a non-singular theory of dislocations (3). Additionally, the segregation energy fields of a single solute towards different GBs have been computed using series of molecular statics simulations. Comparisons were studied between these segregation energy distributions and the distributions given by the different interaction energies. To fully model solute interaction with GB, we highlight the importance to consider, in some situations, the shear stress components of the GB, in addition to the traditionally considered hydrostatic stress. These results bring us one step forward to bridge the scales by contributing to build an improved continuum-based segregation model predicting solute concentration distributions at GBs (4).

References :

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