Responsable :
Martine Logé
☎ 01 69 08 51 67

SEMINAIRE

Service de Recherches de Métallurgie Physique

DEN/DANS/DMN

Bibliothèque du SRMP – Bâtiment 520 – Pièce 109

First Principles Calculations of Point, Line and Planar Defects in Metals

Christopher WOODWARD

Air Force Research Laboratory
Materials and Manufacturing Directorate
Wright-Patterson Air Force Base, Ohio, USA

Here we review property predictions for a variety of defects in metal alloys by means of density functional theory. The emphasis of this work is on defects that mediate or influence plastic deformation such as dislocations, solid solutions, and precipitates. The free energy of relevant point and planar defects are estimated from thermodynamic models based on these first principles results. For example, the site selection and density of ternary solutes in ordered intermetallics (e.g. Al3Sc+X) and the equilibrium profile of interfacial boundaries (IFB) in Al-Al3Sc are estimated using a lattice gas model appropriate for dilute levels of impurities. For Al-AL3Sc+Mg alloys impurity segregation of Mg to the Al side of the (100) IFB is predicted, a result recently verified by atom probe tomography. Alternatively, a cluster expansion method is used to study composition profiles and free energies of IFB's in Ni-Ni3Al. Finally, we have also developed methods for containing the strain field of isolated dislocations (i.e. line defects) in very small simulation cells. Using this technique we have studied the equilibrium strain field of dislocations in bcc (Mo, Ta, Fe), fcc (Al, Ir), and intermetallic alloys (L10 TiAl). We have evaluated solute dislocation interactions in Mo-X (X=Hf, Ta, Re, Os, Ir and Pt) and these interactions are used to inform a new model of solution hardening and softening at low temperatures. Recently, we have evaluated solute-edge dislocation interactions in Al-Mg alloys and differences between the first principles and continuum estimates of the Cottrell "atmosphere" are presented.

Mardi 18 novembre 2008 à 10h30

N.B *: Les visiteurs de nationalité étrangère hors Union Européenne sont priés de bien vouloir avertir impérativement 3 semaines à l'avance – les visiteurs de l'Union Européenne 1 ou 2 jours avant le séminaire – le Secrétariat du Service de leur entrée sur le Centre :*
Tel : 01 69 08 66 64 – Fax : 01 69 08 68 67

Commissariat à l'énergie atomique
SAC/DEN/DANS/DMN/SRMP/Bat 520
91191 Gif-sur-Yvette Cedex - France
☎Tel : 01.69.08.66.64 - Fax : 01.69.08.68.67