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 approach to phase stability, phase equilibria and phase transition for Fe-based binary alloys

Tetsuo MOHRI
Division of Materials Science and engineering,
Graduate School of Engineering, Hokkaido University, Sapporo, JAPAN

We have been attempting a synthesized study of phase stability, phase euilibria and phase transition from the first-principles. The theoretical tools employed are FLAPW electronic structure calculations, Cluster Variation Method (CVM), Path Probability Method (PPM) and Phase Field Method (PFM), and particular focus is placed on Fe-Ni, -Pd and –Pt alloy systems. Spin polarized calculations correctly predict the stability of phases appeared or disappeared in each system, whereas non-polarized calculations destabilize all the ordered phases appeared in the conventional phase diagram. This indicates the importance of magnetism in the stability of Fe-based alloys. L10-disorder phase boundaries are reproduced with high accuracy for Fe-Pd and Fe-Pt systems, while even for Fe-Ni system the present first-principles calculation implies the appearance of the L10 ordered phase. Furthermore, the calculation of the Coefficient of Thermal Expansion provides a clue to understand the invar property which is a characteristic feature of Fe-Ni system.

The extension of the present first-principles study has been attempted to time domain. For this, by combining CVM with PFM, temporal evolution process of antiphase domains associated with L10 ordering process is calculated. Although spatial scale and crystallographic orientation are uniquely fixed, assigning an absolute time scale is left for the future work. The author believes Path Probability Method will play an important role in the determination of the time scale.

Vendredi 30 juin 2006 à 14h

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