DE LA RECHERCHE À L'INDUSTRIE

cea

Séminaire

SRMP

Mardi 15 mars 2016 à 10h30

Salle de réunion du SRMP – Bâtiment 520 - Pièce 109

Modeling the paramagnetic state of magnetic materials from first principles, methods and applications

Björn Alling

Department of Physics, Chemistry and Biology (IFM)
Thin Film Physics Division
Linköping University, Sweden

Many applications of magnetic materials, e.g. Fe-based alloys, take place in the paramagnetic regime above the critical ordering temperature. Furthermore, even when low temperature applications are intended, the materials are typically synthesized in the paramagnetic regime. For these reasons it is valuable to obtain a theoretical methodology for modeling the paramagnetic phase of magnetic materials from first principles. This is a formidable challenge due to the simultaneous presence of magnetic, vibrational, electronic and structural excitations and disorder. In this presentation I will discuss recent methodological development that we have performed of several supercell-based implementations of disordered local moments (DLM) DFT-calculations suitable to address complex materials science problems.

In particular I will demonstrate results obtained with DLM-molecular dynamics (DLM-MD) where the effects of lattice vibrations on e.g. magnetic, and electronic structure of paramagnetic Fe can be directly observed. It is shown that at the high temperature of the gamma-delta transition in Fe, vibrations and magnetic disorder almost completely remove the differences in local magnetic moments and electronic density of states between the FCC and BCC structures. I will also show results of simulations of properties and phase stability in the important paramagnetic hard coating material CrN.

Les visiteurs de nationalité étrangère hors Union Européenne sont priés de bien vouloir avertir impérativement 3 semaines à l'avance, et ceux 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 et aux énergies alternatives
DEN/DANS/DMN Service de Recherches de Métallurgie Physique
Centre de Saclay – Bât. 520 - 91191 Gif-sur-Yvette Cedex – France

Séminaires - Martine Logé ☎ 01 69 08 51 67 et Manuel Athènes ☎ 01 69 08 37 69