Direction de l'Energie Nucléaire – DEN
Département des Matériaux pour le Nucléaire – DMN
Service de Recherches de Métallurgie Physique – SRMP

Postdoctoral research position at CEA-Saclay, France

Modelling the interplay between magnetism and defects in binary Fe alloys

A 24-month postdoctoral position is open in the Laboratory of Physical Metallurgy (SRMP : Service de Recherches de Métallurgie Physique) in CEA-Saclay, in the frame of a french-german ANR-DFG joint research project.

Subject description:

Iron based alloys such as steels play an important role as structural materials for numerous technological applications. For a rational design of these materials, an accurate knowledge of properties of structural defects, and their interaction with impurities and alloying elements in the steels is essential. These properties have a direct impact on the microstructural and mechanical behavior of the materials.

Up to date, extensive theoretical works have devoted to the study of properties of defects in steels, employing quantum mechanics based methods. Most of them are mainly focused on the energetic and kinetic features, such as the stability, mobility and clustering of defects and of solute atoms. However, the iron alloys often show a complex structural-magnetic phase diagram. Many of their properties strongly depend on the magnetic state of the materials. It is therefore necessary to understand and quantify the magnetic effects, including the impact of the magnetic disorder at finite temperatures and the magnetic transitions. The latter features represent a significant challenge from a theoretical point of view, and are currently attracting extensive effort worldwide.

The aim of this postdoctoral work is to investigate the interplay between the magnetism and defects/impurities in a binary Fe alloy, that is, how the presence of defects may change the local magnetic configuration, and how the magnetism may modify the stability, diffusion and segregation properties of point defect, defect clusters and nano-precipitates. The study will focus on bcc Fe-Co and Fe-Cr systems, exhibiting well distinct magnetic-interaction characteristics.

To this end, first principles calculations based on Density Functional Theory (DFT) will be performed to accurately determine the magnetic, energetic and diffusion properties of the binary alloys containing defects, at various magnetic (ordered and disordered) states. Then, effective interaction models, which account for both chemical and magnetic degrees of freedom, will be parameterized using the DFT data. These models, coupled with Monte Carlo simulations will allow studies of magnetic-defect interplay as a function of temperature, and enables to get closer to realistic materials working conditions.

The successful candidate is expected to perform DFT studies and to develop the magnetic effective interaction models.

The salary is around 3100€ per month. The position is available immediately.

Skill requirements:

Applicants should hold a Ph.D degree in Solid State Physics or Materials Science or a closely related discipline, with expertise/experience in Density Functional Theory (DFT) simulations

of magnetic systems. Additional knowledge/experience in programming (e.g. FORTRAN, C, etc.), atomic Monte Carlo and tight binding modelling are considered as a plus.

Contacts:

Chu-Chun Fu
CEA Saclay
DEN/DANS/DMN/SRMP
91191 Gif-sur-Yvette Cedex
France
Tel : + 33 1 69 08 29 32
chuchun.fu@cea.fr

Frédéric Soisson
CEA Saclay
DEN/DANS/DMN/SRMP
91191 Gif-sur-Yvette Cedex
France
Tel : + 33 1 69 08 27 67
frederic.soisson@cea.fr