DIRECTION DES SCIENCES DE LA MATIERE,
INSTITUT RAYONNEMENT MATIÈRE DE SACLAY

SERVICE DE PHYSIQUE ET DE CHIMIE DES SURFACES ET DES INTERFACES

SEMINAIRE *

Vendredi 22 octobre 2010 à 11h00

Bâtiment 466, salle 111 - CEA Saclay, 91191, Gif sur Yvette

Designing a Surface Alloy from First Principles

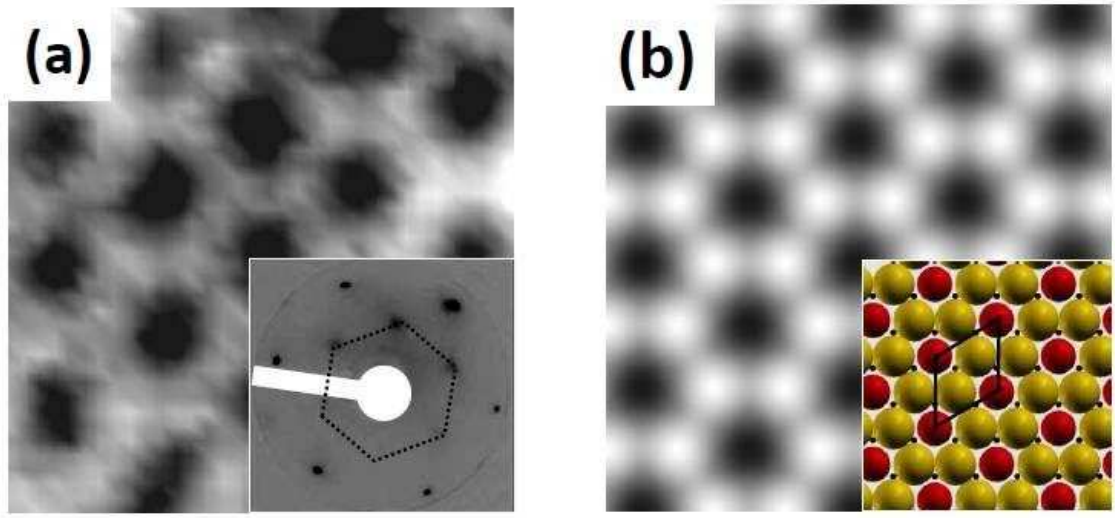
Shobhana Narasimhan

Jawaharlal Nehru Centre for Advanced Scientific Research

Bangalore, India

Invitée par Cyrille Barreteau

In the search for new materials for desired applications, alloying offers a promising way of combining metals to obtain a new material with properties that are different from those of the constituent elements. However, not all combinations of metals are miscible. One way to coax immiscible metals to form an alloy is to deposit them as a thin layer on a substrate. We have performed combinatorial ab initio calculations to study the factors that govern this process, and identified suitable candidates that may behave in the desired way. One of the candidates identified by us, Fe-Au/Ru(0001), has been shown by our experimental collaborators, in the group of Sylvie Rousset at the Universite de Paris - Denis Diderot, to form a stable long-range-ordered surface alloy, even though Fe and Au are bulk-immiscible. Surprisingly, our investigations show that it is magnetic interactions and not stress-relief, that provide the main driving force for mixing in this system.



*** SERA PRECEDE D'UNE PAUSE-CAFE A PARTIR DE 10H30**

Formalités d'entrée : Contacter le secrétariat pour l'établissement de votre autorisation d'entrée sur le centre de Saclay. Tel : 01.69.08.65.32 ou 01.69.08.40.12; Fax : 01.69.08.40.44 ; e-mail : catherine.julien@cea.fr. Le délai minimum est de 24 heures pour les visiteurs ressortissants des pays de l'Union Européenne, et de huit jours pour les autres. Sans autorisation, vous ne pourrez entrer sur le centre de Saclay. Dans tous les cas, se munir d'une pièce d'identité.