Joint modeling of the structure and the properties of magnetic alloys and nanoalloys

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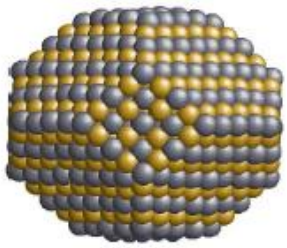
Nanosystems are widely exploited in numerous domains, like magnetic storage, catalysis, or medicine. However, designing a suitable system requires to set an accurate relationship between the properties and structure. Nanoalloys[1] (see figure) are a good answer to this problematics since by combining their finite-size effects with the properties of metallic alloys it is possible to exploit the chemical arrangement inside the particle to build devices with targeted properties. In the nanoalloys, the atomic arrangements (structure and morphology) and the electronic structure should vary with the respective composition of the metals. Controlling the chemical arrangement represents a possible route to tune the properties, as well as their coupling (considering magnetic and catalytic ones for instance).



Typical chemically ordered nanoalloy

For this thesis work, the choice of the systems to investigate has been guided by their ability to exhibit chemical order known to enhance magnetic properties (local magnetic moment and magnetic anisotropy). Thus, materials like CoPt, FePt and NiPt are potentially interesting for their magnetic and catalytic properties. With these model systems, it is proposed to disentangle the respective roles of atomic relaxation, surface segregation, chemical ordering and magnetism in their resulting configurations.

The systems will be studied by using classical atomistic simulations (Monte Carlo, Molecular Dynamics) and density functional theory for the structural and chemical optimization of the systems. **A large part of the study will be devoted to develop a new strategy to model the energetics of such systems while keeping a stronger link to the electronic structure than with usual interatomic potentials[2].** This new model will be built within the tight-binding formalism founded on *ab initio* calculations where magnetism (spin) will be explicitly implemented within a recently achieved procedure[3]. The method will be applied successively to bulk alloys, surface alloys and nanoalloys in an approach of increasing complexity. An extension of the model to C- and H- metal bondings will be explored in order to consider also the systems in realistic environments where foreign (ad)sorption is also modifying the structure and consequently the properties. Interactions with other research groups in the field of «modelling materials» will be provided through the participation to the activities of the french network GDR ModMat (http://www.cinam.univ-mrs.fr/site/modmat/).

Interest in computational physics is recommended for this project.

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1 R. Ferrando R, Structure and Properties, vol. 10, 1rst edition, Elsevier, 2016.

2 F. Cleri et V. Rosato, *Tight-binding potentials for transition metals and alloys*, Phys. Rev. B 48, 22 (1993); H. Sheng, M. Kramer, A. Cadien, T. Fujita et M. Chen M, *Highly optimized embedded-atom-method potentials for fourteen fcc metals*, Phys. Rev. B 83, 134118 (2011).

3 C. Goyhenex, G. Tréglia, B. Legrand, *Environment dependence of magnetic moment and atomic level shifts within tight-binding approximation: An illustration in the case of cobalt*, Surf. Sci. 646**,** 261 (2016).