Modeling of metallic nanoalloys at the atomic scale

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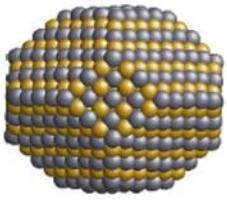
Nanoparticles of alloys or nanoalloys are nowadays the subject of a great amount of studies because of their numerous potential applications in magnetic storage, catalysis and biotechnologies [1]. On a theoretical point of view, a large number of properties of the perfect bulk metallic alloys are accessible to *ab initio* calculations like the cohesive energy, the elastic properties, the magnetic properties or the energy formation of ordered phases and of simple defects like a surface or a vacancy. However, when dealing with extended defects (like grain boundaries) or nanoparticles of a few hundreds or thousands of atoms it becomes very difficult to simulate their structure and their chemical ordering properties because the sizes of the systems under study are too large and it would require a too long computer time. Even for reasonable sizes it remains very computer time demanding to characterize their evolution as a function of time and temperature. For these reasons, atomistic simulations, classical Molecular Dynamics and Monte Carlo, are performed. They mainly require an interatomic potential sufficiently reliable but at the same time sufficiently simple.

We have recently proposed a new methodology for overcoming this important scientific challenge and for enabling the study of complex (nano)alloys, starting from *ab initio* calculations. From such ab initio calculations on pure metals (ideal bulk) and of ordered phases of alloys (bulk), a tight-binding potential, with an adjustable complexity (method of moments), is under development in order to reproduce at best these *ab initio* results. A crucial point in this development is to include the part of the energy due to magnetism which is not done in the usual potentials. A treatment of the magnetism has been recently proposed based on a self-consistent treatment starting from non-magnetic local densities of states [2].

In this context the master student will test this treatment in the case of CoPt alloys in the aim to find the energy formation of ordered phases of the alloys, to characterize the local magnetic properties of the same alloy in the presence of a surface and finally in an ordered CoPt nanoparticle (see figure). The project will require writing a simple code preferentially in FORTRAN.



Example of an ordered nanoparticle with a regular arrangement of two metallic species alternating pure planes of a metal A and a metal B represented by two different colors.

References:

[1] R.L. Johnston and R. Ferrando, Nanoalloys: from theory to application, Faraday Discussions 138 (2008) 9

[2] C. Goyhenex, G. Tréglia and B. Legrand, Surf. Sci., in press DOI : 10.1016/j.susc.2015.09.004