204 Subnanoscopic Co and CoNi cylinders

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One of the most convenient shapes among magnetic nanoparticles is the cylindrical, and they can be solid [1] or hollow [2]. They are easy to produce in different sizes at the nanoscale, a variety of elements and compounds have been tested, they get axial magnetization due to their geometrical anisotropy, and they are relatively easy to handle. The search is focused along several directions at present, one of which is to make these particles as small as possible.

Which is the minimum stable cylindrical shape possible? How stable are they? Can they grow from a seed to make large particles? What are their physical properties at this scale where quantum mechanics operate? How do they compare with the usual magnetic nanocylinders usually described by means of classical magnetism?

Some of these questions have been recently answered for the case of cylinders formed by Co atoms [3]. In this presentation we want to get deeper into this problem in particular considering binary magnetic alloys like it is the case when Ni atoms substitute for Co in the original stable structures.

In Fig. 1 we present a particle formed by 17 atoms: 2 of them are on the "vertical" axis and the remaining 15 are at the vertices of three pentagons intercalated with previous single atoms on the axis. Such structure is stable and can be extended along the axis. An insulator-metal transition was found for a critical length of such wire and the magnetization was found to increase from the center towards the end of the cylinder [3].

Here we consider the case in which Ni atoms substitute for Co at several positions: on the axis, on the mantle, on the rim. The last case is shown for 2 Ni atoms in Fig. 1. Several other compositions and combinations will be calculated in the analysis. Program SIESTA is invoked to minimize energy of the configuration using standard procedures.

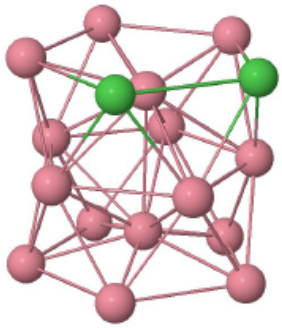

Fig. 1 *A magnetic nanopillar constituted by 17 Co atoms (if different colours are ignored) or constituted by 15 Co atoms and 2 neighboring Ni atoms on the rim (if different colours are considered).*

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References

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