Tailoring Structure of Bimetallic Nanoparticles by Coalescence and Size Effects

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Bimetallic supported magnetic nanoparticles have received considerable attention because besides the size reduction effect, the addition of a second metal provides a method to control their properties and functionalities through a tailoring of their structure. Because the determination of atomic structure at the nanoscale is a complex problem, methods that probe local and average NPs features as well as nanometer to micrometer-sized data, provide highly complementary information about the structure and morphology of nanostructures and are much powerful when used together. For that, we have used simultaneously Grazing Incidence Small-Angle X-ray Scattering (GISAXS) and Grazing Incidence X-ray wide angles scattering (GIWAXS) in UHV conditions¹, which allow the determination of the structure at the atomic scale range (small angles) and the morphology at the particle scale range (wide angles), respectively. The quantitative structural analysis have been facilitated and consolidated using Monte Carlo (MC) simulations² of CoPt nanoallovs within a semi-empirical tight-binding potential (fig. 1). During the annealing or in-temperature growth experiments (from 300 to 900 K), the in situ scattering measurements were carried out on two different surface diffractometers on both ID03 and BM32 beamlines using an ultrahigh vacuum setup^{1,3}.

On weak interacting substrates (disordered silicon oxide or amorphous carbon sublayer), the challenge is to distinguish during the internal atom rearrangement induced by thermal treatments, between the atom-by-atom mobility and the large motion of atoms induced by the coalescence, which lead to crystalline (ordered or disordered) or multitwinned (icosahedral, decahedral) nanoparticles³ (fig. 1). At these substrate temperatures, some kinetic effects (aggregation-coalescence) can induce atomic rearrangements leading to large structural change, far from the equilibrium state, while the atom diffusion in size-stabilized particles leads to structures in agreement with thermodynamic equilibrium calculations. Finally, recent in situ and ex situ scattering experiments on core-shell supported nanoparticles will presented.



Fig. 1: GIXD patterns obtained at increasing annealing temperatures and corresponding simulated pattern calculated from Monte Carlo simulations (Ih icosahedral a), Dh decahedral b) and disordered/ordered TOh c–d) clusters).

References

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