PhD third year report

PhD student: Nicolò Canestrari

Tutors: Riccardo Ferrando, Diana Nelli

1 Research Activity

My research activity is within the Nanobiocomp research group, where we investigate the behaviour of matter at the nanoscale by computational tools. In my work I mostly apply molecular dynamics (MD) simulations to the study of nanoparticles and nanoalloys, with regard to the different structures and processes of growth and diffusion.
It is possible to describe within a general theoretical framework all the different kinds of icosahedral multi-component aggregates, which should help the design and realization of new metal nanoparticles with desired properties for a huge variety of applications [1]. A great part of the work of MD simulations done to validate this framework, particularly the successfully simulated growth of bimetallic nanoparticles with chiral and achiral layers, has been published in the research article. This includes most of the simulations done with the binary systems Ni@Ag, Co@Ag and Cu@Ag. Also as part of mapping and explaining all possible icosahedral nanoparticles, two MD growth simulations of an antimackay/pentakis icosahedron have been included, both with the complete realization of the aggregate and with a resulting chiralization.
Beginning with the Ni@Ag chiral icosahedron, a general exploration was made of homogeneous diffusion on all Ag (111) surfaces, considering also the mackay icosahedron, the octahedron and the tetrahedron [2]. The diffusion process was studied in two ways: by adding an Ag atom on the surface, running an MD simulation and then taking an Arrhenius plot; and by taking a profile of potential energy with very slow changes of the relevant coordinate ('drag method'). The two methods gave very consistent results with the icosahedra, while some discrepancy was observed when the energy barrier for moving between facets of the nanoparticle was comparable to the one for moving on the facet. Mass mobility on the nanoparticle can be due to 'jumps' from one facet to the next as well as 'exchanges' when the moving

atom takes a place on the edge and send the atom that was there on the other facet. The main result of this investigation is that both the smoother surface, the chiral icosahedron, and the sharper one, the tetrahedron, have the higher mass mobility, with the two mechanisms of 'jump' and 'exchange' prevailing respectively on the smoother and sharper surface. The same pattern was also observed for Cu (111) surfaces.
A study was made of pressure within both a crystalline structure such as the octahedral nanoparticle and a non crystalline one as the (mackay) icosahedral one. We considered in particular the pressure on the central atom due to the forces between it and the near neighbours, and calculated it with our usual atomic potentials for both Ag and Cu nanoparticles. While we were able to verify the Laplace law for the octahedron and a power law with a positive exponent for the icosahedron (due to a central field), the data were not in agreement with the expected surface tension for both metals.

2 Exams

Exam given: Theatrical techniques for scientific presentations (by Antonio Sgorbissa): 3 cfu.

3 Poster contributions

Poster contribution "Icosahedra: structure and growth" presented at the conference 'Cluster Meeting 2025' in Prague.

4 References

[1] Nicolò Canestrari, Diana Nelli, and Riccardo Ferrando. "General theory for packing icosahedral shells into multi-component aggregates." Nature Communications (2025): 16, 1655.
[2] Nicolò Canestrari, Riccardo Ferrando, and Diana Nelli. "In search of the smoothest nanoparticle surface: diffusion and mobility on Ag clusters." Nanoscale (2025): 17, 16784.