PhD first year report

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1 Research Activity

I work as part of 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, and particularly of the process of growth.

My first PhD year has been devoted to the study of a new kind of core-shell nanoparticle: an icosahedral (of the Mackay type) core of atoms of one metal species surrounded by many chiral layers of a different one (a chiral multilayer), leading also to new magic numbers. The initial purpose was to verify by MD simulations the recovering of an anti-Mackay arrangement already predicted by global optimization searches for Cu@Ag nanoparticles. Then, simulating growth in an Ni@Ag bimetallic system, we observed this new chiral multilayer configuration, given certain conditions, and particularly when Ag atoms were added on a big enough Ni core. This result was then extended to other bimetallic systems, always using a similar choice for the inter-atomic potential (second moment tight binding): other similar results were obtained for Co@Ag, Co@Au, Ni@Au, Cu@Ag and finally Fe@Au, depending on the size of the initial seed. Depending on the system, we also observed different degrees of perfection in the resulting chiral multilayer: sometimes there would be more exchanges between the core and the shell, sometimes less or none.

We verified the stability of this arrangement by first making heating simulations and seeing that there is no change in this structure up to the point where melting occurs, and then by conducting a global optimization search, which didn't lend better results except for some completely different configuration. In order to study in more detail the stability of the chemical ordering we collected structures for all these systems and exchanged atoms between the shell and the core, usually resulting in an increase of energy. By doing the same with the corresponding Mackay icosahedra, we showed these to be less

of a stable arrangement for these bimetallic systems. Similarly, a comparison was made between the pressure map of these two configurations and also a comparison in term of energy, adding more atoms to the chiral multilayer in order to have the same number as for the Mackay configuration.

Both the description of the growth of one layer on top of the other, and the understanding of the properties of the surface of this new structure, required us to investigate the diffusion on the surface of the chiral multilayer. We made MD simulations of one atom on top of the shell (of the same atomic species) by which we came to quantify the smoothness of the chiral multilayer's surface, making an Arrhenius plot of the number of jumps from one facet of the nanoparticle to the next at different temperatures. The same result was obtained by local minimization (quenching) applied to the atom along its path from one facet to the next (drag method). These results, which will be included in the publication, are also relevant to possible catalytic uses, and may be the object of a DFT calculation in the continuation of this work.

We also observed for the different systems and sizes that this structure is better at packing atoms, which lead us to investigate its nature, also in order to be able to build a prototype of a given size with a simple program. This is possible by considering this as part of the family of icosahedra already described by Caspar and Klug in their work on viruses. This is the point where a scientific article is being refined in order to arrive soon at a publication.

2 Courses and exams

FISICA STATISTICA DEI SISTEMI FUORI EQUILIBRIO (by Nicodemo Magnoli).

Atomic force spectroscopy (by Annalisa Relini).

Advanced Computational Physics (by Riccardo Ferrando, Diana Nelli): exam given.

Paris International School on Advanced Computational Materials Science (PISACMS 2023): exam given.

3 Conferences and contributions

Poster contribution "Simulated Growth of Ag and Au Chiral Shells on Icosahedral Seeds" presented at:

International Meeting on Nanoalloys 2023 in Orléans

PISACMS 2023 in Paris.

CMD30 FISMAT 2023 in Milan.