PhD report

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Research activity

Here I describe the results obtained during my second year as a PhD student. Most of my activity was dedicated to the study of metallic nanoparticles by means of computer simulations and Machine Learning algorithms. In particular, the core of my work was the research of a more efficient way for describing and clustering nanoparticles in different structural families, than that already studied and published during my first year. To do so, I implemented a scheme which can be divided in three main parts. The first one relies on a very detailed description of nanoparticles based on the Common Neighbor Analysis. Thanks to this tool, each nanoparticle can be described with a 64-dimensional vector which embeds the information regarding the local environment of each atom. The second step is a reduction of the dimension of this vector in order to better visualize and to make easier the application of clustering algorithm. This was done thanks to the Principal Component Analysis, which is a standard algorithm for the problem of dimensionality reduction, and it is well known for its capability of preserving a certain amount of the variance of data. The third and final step is the application of an unsupervised learning algorithm together with a score metric for clustering the nanoparticles in this reduced space. I found that the Gaussian mixture model together with the Bayesian information criterion is the best choice for the pursuit of such result. Thanks to this choices, I was able to obtain good results even on complicated data sets involving disordered structures obtained for example from molecular dynamics simulations of nanoparticles evolution at high temperature. The work is now under submission [4].

Together with Dr. Minnai (Experimental Physicist at the Okinawa Institute of Science and Technology) and Dr. Nelli, from our group, we wrote a review about the role of strain in metallic nanoparticles. This work, which is now under submission, encompasses different experimental and theoretical results about the influence of strain on various properties (structural, chemical, optical, magnetic). It aims at making a resource as complete as possible about this topic which is of primary importance in the field of nanoalloys.

I was also involved in other research project of my group. The first one is that of ref. [1]. In this work we studied two similar bimetallic systems, namely AuAg and PtPd nanoalloys, by means of molecular dynamics simulations. These two systems, which are of some interest due to their applications in catalysis and plasmonics, are very similar because there is a little size mismatch between the two elements and a tendency towards surface segregation for the less cohesive element. Our aim was then to single out the differences that occur in growth simulations (where atoms are deposited on the surface of the nanoparticle, a situation which is close to gas phase experiment) at different temperatures. First, we showed that the chemical ordering obtained in our simulations is the same of experiments, then we analyzed them in further detail and we discovered some differences. In particular we found that the migration of Ag and Pd in simultions in which they are minority elements is stronger that that found when Au or Pt are. Moreover, we found that this mobility is a little stronger for Ag than Pd.

Another work in which I collaborated was that of ref. [1]. Here, we studied and solved a long-standing open problem about the growth of Au nanoparticles. In particular, it is experimentally well-known that some of these nanoparticles grow from a tetrahedral motif to a decahedral or icosahedral one, the mechanism being unknown. Thanks to molecular dynamics we could reveal the physics phenomena behind this process, at atomic level. Thanks to growth simulations, we found that starting from a tetrahedral seed, the key mechanism towards a decahedral motif takes place in two stages: (i) the formation of metastable islands in stacking fault on the surface facets of the tetrahedral seed and (ii) the stabilization of these islands thanks to other layers growing on top of them. After this, there is place for a fivefold axis to grow, and so the pathway from tetrahedral seed towards decahedra or icosahedra can be understood. In order to strengthen our conclusions, we also performed some Density Functional Theory (DFT) calculations.

List of publications

[1] El Koraychy, E.; Nelli, D.; Roncaglia, C.; Minnai, C.; Ferrando, R. Growth of size-matched nanoalloys - a comparison of AuAg and PtPd. *Eur. Phys. J. Appl. Phys.* **2022**, *97*, 28. `https://doi.org/10.1051/epjap/2022210297`

[2] El Koraychy, E.; Roncaglia, C.; Nelli, D.; Cerbelaud, M.; Ferrando, R. Growth mechanisms from tetrahedral seeds to multiply twinned Au nanoparticles revealed by atomistic simulations. *Nanoscale Horiz.* **2022**, *7*, 883-889. `https://doi.org/10.1039/d1nh00599e`

[3] Roncaglia, C. Gaussian mixture model for the unsupervised classification of AgCu nanoalloys based on the common neighbor analysis. *Eur. Phys. J. Appl. Phys.* **2022**, *97*, 11. `https://doi.org/10.1051/epjap/2022210262`

[4] Roncaglia, C; Ferrando, R. Machine Learning Assisted Clustering of Nanoparticles Structures. Currently submitted at Journal of Chemical Information and Modeling.

List of attended schools and conferences

I was in the organizing committee of the following conference in Santa Margherita Ligure, Genova (Italy), where I also presented a poster.

- Cluster-Surface Interaction Workshop 2022 (April 1-4, 2022). Link: `https://csi2022.unige.it/`

I attendend the following school in Cargèse, Corsica Island (France), where I also presented a poster.

- Spring School on Nanoalloys. From Structure, Kinetics and Environment, to Properties and Applications. (April 24-30, 2022). Link: `https://nanoalloys-irn.cnrs.fr/spring-school-on-nanoalloys-2022/`

Visits

- I visited Prof. Hauser at the Physics Department of Graz University of Technology from May 28 to June 4, to collaborate on our project about the definition of an atomistic potential for PtNi and AuNi nanoalloys through Machine Learning techniques. Work is in progress.

- As a group, we visited Prof. Pietrucci at the Physics Department of Sorbonne University, in order to develop the scientific collaboration between our groups. Our aim is the combined approach of computer simulations and statistical mechanics for the study of metallic nanoparticles. We also visited Prof. Andreazza at the laboratory "Interfaces Confinement Matériaux Nanostructures" (ICMN) at Orléans, France, for a collaboration on the study of nanoalloys.