Diana Nelli

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Annual report of the activity during the year 2018/2019

Research activity

The aim of my research activity is the study of equilibrium and out-of-equilibrium properties of nanoparticles and nanoalloys by computational methods. During this year I have worked on three main topics:

- Evolution of bimetallic nanoalloys at constant temperature from out-of-equilibrium randomly intermixed configurations

  In synthesis experiments, nanoparticles are often produced in out-of-equilibrium configurations; they then evolve towards equilibrium undergoing changes in their geometric structure and, in the case of nanoalloys, in their chemical ordering, and their properties change accordingly. The study of this equilibration process is thus of great interest, both on the experimental and theretical level. We have studied the evolution of AuCo, AgNi and AgCu nanoparticles from randomly intermixed configurations to the equilibrium phase-separated core-shell configuration; we have performed long-scale molecular dynamics simulation at different temperatures from 300 to 700 K. The aim of this work was to track the possible evolution pathways (i.e. the configurations explored during the evolution) and to compare the pathways obtained for the three systems. The results obtained have been published (see the list of publications below) and presented at various conferences (see list of contributions at conferences).

- Coalescence of gold nanoparticles at constant temperature

  Coalescence is often an important step in the growth of nanoparticles; in this process two preformed clusters collide and merge to form a larger aggregate, whose shape evolves from an initial configuration, which is typically strongly out-of-equilibrium, towards more compact structures. We have studied the coalescence of Au clusters by long-scale molecular dynamics simulation at 400 and 500 K. The aim of this study was to follow the evolution pathways of the coalescing aggregate, i.e. whether the equilibium structure is reached or not and which type of intermediate configurations are obtained. In particular we studied the influence of the geometric shape of the colliding units and their mutual orientation on the evolution process. This work has been done in collaboration with the experimental group of Richard E. Palmer (Swansea University, UK), which provided TEM images of gold nanoparticles during the coalescence process. The results obtained have been submitted (see the list of publications).

- Evolution of bimetallic nanoparticles from metastable configurations by advanced computational techniques

  During the evolution of nanoparticles towards thermodynamic equilibrium, metastable configurations with very long lifetime are sometimes reached; this behavior leads to long equilibration time scales, ranging from seconds to minutes or even months. The computational study of such evolution may be quite challenging: standard molecular dynamics techniques can only reach time scales up to some microseconds for nanoparticles of sizes of a few thousand atoms, therefore is necessary to develop advanced techniques, such as metadynamics, to extend the time scale of the simulations. We use a recently developed form of metadynamics to study the evolution towards equilibrium at room temperature of AuCo nanoalloys of diffeent sizes and compositions. This work is carried out in close collaboration with dr. Fabio Pietrucci (IMPMC, Sorbonne University, Paris, France).

Publications

- D. Nelli and R. Ferrando, *Nanoscale*, 2019, **11**, 13040 – 13050

  Title: "Core-shell vs multi-shell formation in nanoalloy evolution from disordered configurations"

- D. Nelli, G. Rossi, Z. Wang, R. E. Palmer and R. Ferrando, *submitted*

  Title: "Memory effects in the coalescence of Au clusters"

Oral contributions at conferences

- International Meeting on Nanoalloys, IMN 2019

  Genoa, Italy, June 4-7, 2019

  Title: "Core-shell vs Multi-shell Formation In Nanoalloys Evolution From Disordered Configurations"

- CECAM Workshop "Modeling metal nanoparticles: environment and dynamical effects"

  Grenoble, France, December 3-5, 2018

  Title: "Structural transformations in AuCo nanoalloys studied by metadynamics"

Poster contributions at conferences

- Advances in Cluster Beam Deposition

  Okinawa, Japan, October 21-25, 2019

  Title: "Transformation pathways in out-of-equilibrium nanoalloys: from randomly mixed, to three-shell and core-shell structures"

- Cluster and Nanostructures Gordon Research Conference "Properties and Functionalities of Nanometer and Sub-Nanometer Sized Quantum Objects"

  Les Diablerets, CH, June 16-21, 2019

  Title: "Competition between core-shell and multi-shell structures in nanoalloy evolution from non-equilibrium configurations"

- International Meeting on Nanoalloys, IMN 2019

  Genoa, Italy, June 4-7, 2019

  Title: "Structural Transformations in AuCo Nanoalloys Studied By Metadynamics"

Conferences organization

Member of the Organizing Committee of the International Meeting on Nanoalloys, IMN 2019 (Genoa, Italy, June 4-7, 2019)

Attended courses

- Quantum Optics
- Advanced Computational Physics (exam passed)
- Elementary Electronic Structure of Solids
- Basic Scanning and Transmission Electron Microscopy (exam passed)

Attended Summer Schools

PISACMS 2019: Paris International School on Advanced Computational Material Science

Paris, France, August 25 – September 1, 2019

I ranked second in the "Best Poster Competition" (title of the poster: "Chemical ordering transformations in nanoalloys studied by molecular dynamics and metadynamics")