SHORT TERM SCIENTIFIC MISSION (STSM)
SCIENTIFIC REPORT

This report is submitted for approval by the STSM applicant to the STSM coordinator

Action number: CM1405 – Molecules In Motion (MOLIM)
STSM title: On the correlation between core positioning and structural stability of Ni-Au core-shell nanoparticles
STSM start and end date: 20/1/2019 to 3/2/2019
Grantee name: Martin Schnedlitz

PURPOSE OF THE STSM:

The main purposes of the STSM were (1) to get the 'know-how' in running large-scale LAMMPS simulations of core-shell Ni-Au nanoparticles; (2) to correlate the results from these simulations (diffusion of Ni atoms and mixing process at the solid phase as a function of time) with the experimental measurements; (3) to represent the data generated by the Madrid group from very long (up to a few hundred ns) simulations in a way that can be intuitively interpreted.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

Having acquired the 'hands on' training on LAMMPS simulations through several test runs, long term molecular dynamics (MD) simulations describing diffusion mechanism of Ni-Au core-shell particles were carried out. In order to validate the experimental results and differences in diffusion mechanism of a centralized and a decentralized Ni cores inside a Au shell, several MD runs for various Ni core positions have been performed.

The second working part focused on the evaluation of diffusion runs, with the goal to calculate descriptive quantities which explain the differences in the diffusion times. This was found to be the mean change in radial distance of all Ni atoms to the center of mass of the bimetallic nanoparticles.

Finally also some testing runs with different core materials (e.g. Cobalt) were performed as well as some simulations with different time steps in the MD simulation.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

The main achievement was in conceiving the idea of how to correlate the experimental outcome on the long-time stability of Ni-Au decentralized nanoparticles with LAMMPS simulations of diffusion of Ni atoms in centralized and decentralized nanoparticles. Specifically, the key idea was to represent the mean average distance of Ni atoms to the center-of-mass as a function of time. While, for the centralized NP, it converges very rapidly, the distance is very 'hardly' modified for the centralized NP. The reason is on the the tendency of the nickel atoms to be located in the subsurface region of the nanoparticle. For the case of the decentralized particle, the nickel atoms are already in contact with this sub-surface area and, then, they diffuse primarily throughout that area. Contrarily, the centralized nanoparticle diffuse through the bulk of the gold phase to reach the subsurface, allowing a faster mixing.

It is expected that the know-how acquired can be transferred to other projects of the Graz group such as that centered on core-shell Co-Au nanoparticles.

FUTURE COLLABORATIONS (if applicable)

Besides completing a joint paper on the studied core-shell NiAu nanoparticles, there are plans in a joint work on simulation the oxidation of the core-shell nanoparticles.