Molecular Dynamics approach to plasma nanoparticle growth and reactivity.

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Controlling catalyst nanoparticle growth is of paramount importance for improving catalyst size distribution, structure and morphology to achieve high activity and selectivity. Experimentally, Magnetron Sputtering - Gas Aggregation Source is a new tool for designing nano(alloy)catalysts [1] based upon plasma sputtering at high pressure in an inert plasma (Ar) or reactive plasma (Ar with O_2, N_2) which is carrying the grown cluster to a substrate through a nozzle.

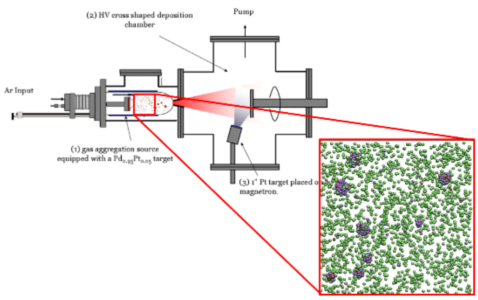

Fig. 1 : Schematics of a plasma condensation source. Inset gives the nanoalloy growth process in the condensation chamber. (after Ref. 1)

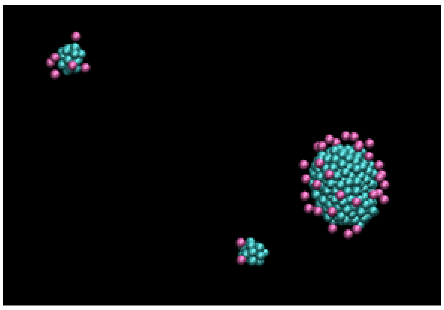

FIG. 2: *Example of Pt_9Bi_1 nanoparticle growth in plasma condensation source. Background Ar gas atoms are removed for clarity.*

Initial conditions of MD simulations are selected for matching experimental chemical and physical Magnetron Sputtering - Gas Aggregation Source parameters. This takes into account the sputtering properties for determining the initial ratios between sputtered and background gas (reactive or not) atoms. Results concerning the growth of $Pt_xNi_yAu_z$, Pt_xBi_y (Fig. 2) and Pd_xO_y nanoparticles under such conditions will be presented. Radial distribution functions and X-Ray Diffraction patterns are systematically computed for enabling direct comparison with experiments.

This work is partly funded by ANR project ECO-PLAN under grant ANR-16-CE29-0007 and by EC FCH-JU SMARTCat under grant GA325327

REFERENCES

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