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 O₂, N₂) 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 PtₓBiᵧ 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 PtₓNiᵧAu₂z, PtₓBiᵧ (Fig. 2) and PdₓOᵧ nanoparticles under such conditions will be presented. Radial distribution functions and X-Ray Diffraction patterns are systematically computed for enabling direct comparison with experiments.

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REFERENCES