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Molecular Dynamics simulations of plasma sputtered nanocatalyst growth

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On one hand, Pt based alloys are known to improve the activity and stability of PEMFC's catalysts [1,2]. On the other hand, magnetron sputtering deposition has already demonstrated its ability for the fabrication of efficient PEMFC electrodes with high Pt utilization rate [3]. In the present study, MD simulations on PtxMyNz (M, N, being less noble or common metals) deposition and growth are carried out for studying the preferred morphology and structure (size, geometry, atomic arrangements ...) of such clusters.
Recently, it has been shown that MD simulations allowed confirming and predicting the morphology and structure of Pt nanocatalysts [4,5] as well as of PtxPdyAuz nanomaterials [6], for which, a comparison is provided between sputtering and chemical methods.
Initial conditions of MD simulations are selected for matching experimental chemical and physical synthesis methods of nanoparticles. MD simulations of catalyst PtxPdyAuz, PtxNiyAuz, and PtxBiy, supported on porous carbon mimicking fuel cell gas diffusion layers as well free nanocluster growth in conditions mimicking gas condensation nanocluster source are studied. Radial distribution functions and X-Ray Diffraction pattern are systematically computed for enabling direct comparison with experiments.
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