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Understanding ternary PEMFC nanocatalyst atomic arrangement during growth and annealing: a Molecular Dynamics approach.

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On one hand, Pt based ternary 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 $Pt_xM_yN_z$ (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..
As the nanoparticle growth by sputtering methods is atomic by nature, simulations at the molecular level are expected to be relevant for understanding basic mechanisms of this deposition method. Indeed, molecular dynamics (MD) as being able to exactly calculating the trajectory of atomic systems is a suitable method for addressing this topic, especially in the context of plasma sputtering [4, 5]. Very recently, it has been shown that MD simulations allowed confirming and predicting the morphology and structure of Pt nanocatalysts [6,7] as well as for $Pt_xPd_yAu_z$ [8]. For the latter, a comparison is provided between sputtering and chemical synthesis methods.
Initial conditions of MD simulations are selected for matching experimental chemical and physical methods. Ternary catalyst $Pt_xPd_yAu_z$, $Pt_xNi_yAu_z$,, $Pt_xCu_yAu_z$ and $Pt_xNi_yCu_z$ supported on porous carbon mimicking gas diffusion layers are studied. Radial distribution functions and X-Ray Diffraction pattern are systematically computed for enabling direct comparison with experiments.

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REFERENCES

1. S. Lankiang, M. Chiwata, S. Baranton, H. Uchida, C. Coutanceau, Electrochim Acta 182 (2015) 131-142.
2. V. Tripkovic, H. A. Hansen, J. Rossmeisl, T. Vegge, Phys Chem Chem Phys 17 (2015)11647-11657.
3. M. Mougenot, A. Caillard, P. Brault, S. Baranton, C. Coutanceau, , International Journal of Hydrogen Energy 36 (2011) 8429-8434
4. P. Brault and E. Neyts, Catalysis Today 256 (2015) 3-12
5. E. Neyts, P. Brault, Plasma Processes and Polymers (2016) DOI: 10.1002/ppap.201600145
6. P. Brault, A. Caillard, C. Charles, R. Boswell, D. B. Graves, Appl. Surf. Sci. 263 (2012) 352-356
7. L. Xie, P. Brault, C. Coutanceau, J.-M. Bauchire, A. Caillard, S. Baranton, J. Berndt, E. Neyts, Appl. Cat. B, 62 (2015) 21 - 26
8. P. Brault, C. Coutanceau, P. C. Jennings, T. Vegge, J. Berndt, A. Caillard, S. Baranton, S. Lankiang, International Journal of Hydrogen Energy 41 (2016) 22589 - 22597