Platinum one dimensional nanostructured catalyst: structural and performance insights

Amra Peles, Anais Espinal, Michael Humbert, Jacquelynn Garofano

United Technologies Research Center, East Hartford, CT 06118

One-dimensional metal nanostructures have attracted a lot of applied and fundamental research interest due to their unusual, non-bulk-like structure and physical properties. They are viable candidates for applications as nanoelectronic devices, mechanically enhancing composites and as industrial catalysts.

Geometric and electronic effects play decisive role for the performance of nanostructured materials in general and catalysts in particular [1] Changes in the types of reaction site, their coordination number with neighboring atoms and the strain at the reaction site profoundly influence their reactivity. Shape, size and stability of nanostructured catalyst affect the overall utilization in technical applications. [1,2] Pt nanowire and nanorods have less low coordinated sites and edges; the surface available for the reaction is much smoother then in particles of comparable diameter which makes these nanostructure viable alternative to the state of the art Pt/C.[2,3]

Here we report on the improvements in the per site activity. We provide an insight into the underlying mechanism of catalytic activity enhancement based on multi scale approach using the first principles Density Functional Theory (DFT) and Molecular Dynamics (MD) calculations and compare with experimental structural and performance characterization. Our approach is based on examining theoretical descriptors of catalyst behavior. Parameters that correlate with catalytic activity changes include electronic structure effects, described by the mean energy of d-band electrons; effect of size, shape and exposed crystallographic orientation. The structural and performance characterization of smooth 1D catalyst will be presented. The comparison of the simulation results with experiments will be discussed as well.

References

[1] Shao M, Peles A, Shoemaker K "Electrocatalysis on platinum nanoparticles: particle size effect on oxygen reduction reaction activity", Nano Letters 11(9), 3714-3719 (2011)

[2] Koenigsmann C, Zhou W , Adzic R R, Sutter E, and Wong S S, "Size-Dependent Enhancement of Electrocatalytic Performance in Relatively Defect-Free, Processed Ultrathin Platinum Nanowires", Nano Letters, 10(8), 2806-2811 (2010).

[3] Koenigsmann C, Sutter E, Adzic R R, and Wong S S, "Size and Composition-Dependent Enhancement of Electrocatalytic Oxygen Reduction Performance in Ultrathin Palladium-Gold (Pd1-xAux) Nanowires", J. Phys. Chem. C, 116(29), 15297-15306 (2012).