Short Communication

Influence of Annealing on Pt Electrocatalyst: Theoretical Approach to Estimate CO Tolerance

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doi: 10.20964/1104311

Received: 31 January 2016 / Accepted: 7 March 2016 / Published: 1 April 2016

For electrocatalytic energy hydrogen systems such as fuel cell (FC) and hydrogen compression there is a demanding requirement for the hydrogen purity. There is a vast opportunity to produce hydrogen from various sources, including fossil fuels; however, in many cases such hydrogen will contain various impurities, such as CO. In our previous work we showed that annealing of a catalyst affects its CO tolerance. Using the same theoretical model for investigating CO tolerance of a catalyst, we explored how temperature of annealing affects CO poisoning of a platinum whiskerette, a nanoobject of an extended-surface support, such as 3M nanostructured thin film (NSTF), or other structures produced by, for example, glancing angle deposition (GLAD) methods, etc. Here we present results of molecular dynamic (MD) modeling of the whiskerette as a model of extended structure annealed at temperatures from 400 to 1200 K. We found that CO coverage increases with annealing temperature, that is, at high temperatures there are more deformations which lead to high CO coverage. Interestingly, we observed sharp peak of CO coverage at temperature above 1000 K. Obtained results suggest range of optimal annealing temperatures.

Keywords: CO tolerance, extended-surface support, annealing, molecular dynamics

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