Early Stages of Carbon Nanotube Growth on Ni nanoparticles: a study of surface reconstruction

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Abstract

Carbon adsorption on various Ni surfaces is investigated as a function of coverage via a combination of first-principles simulations and field emission microscope experiments [1]. It is found that carbon can be efficiently stored as subsurface carbides, but with different energetics on differently oriented surfaces depending on their compactness and density of adsorption sites. In the resulting morphological reshaping,{113} facets are predicted to grow at the expense of {111} and {100} facets, in excellent agreement with experimental observations (see Figure 1). Moreover, at high coverage on the {113} surface the carbon adsorption energy passes through a maximum after which a structural crossover is realized such that carbon atoms tend to ascend to the surface to form one-dimensional chains (which are the precursors of graphitic nanostructures). This rationalizes the experimental observation of an incubation time between carbon storage and the beginning of catalytic growth, and provides insight into the early stages (nucleation mechanism) of carbon nanotubes on Ni nanoparticles.

[1] Y. Wang, G. Barcaro, F.R. Negreiros, T.V. de Bocarmé, M. Moors, N. Kruse, M. Hou, A. Fortunelli, Chem. Eur. J. 2013, 19, 406 – 413

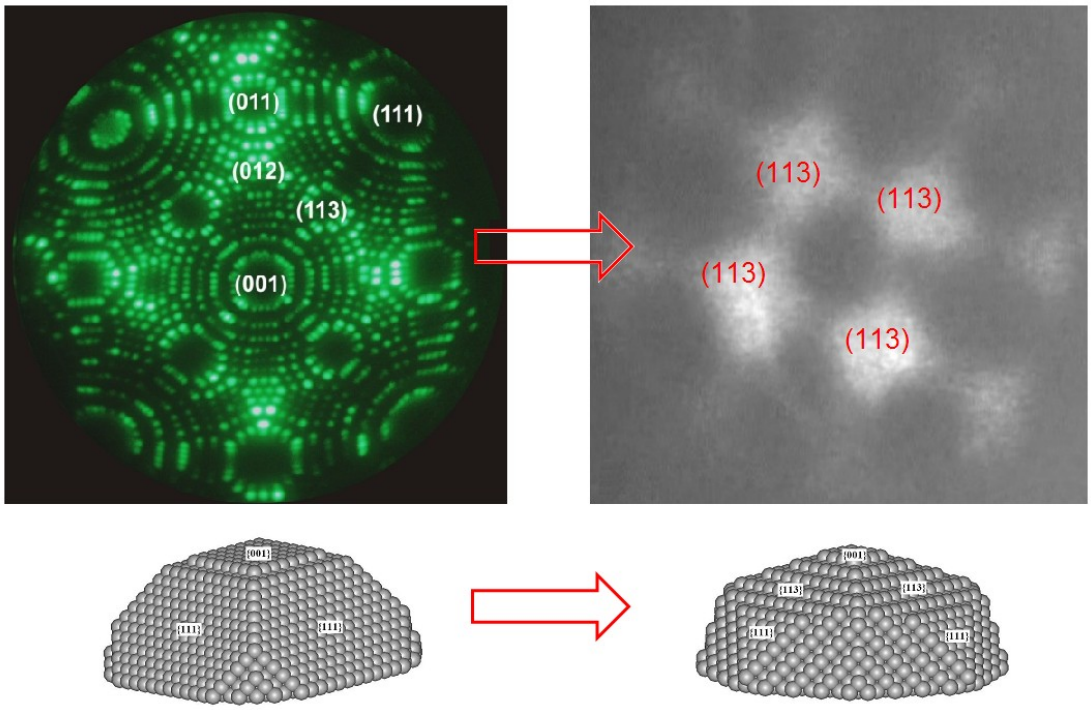

Figure 1: Experimental and theoretical predicted morphology of Ni particles in the case of: a clean surface (left) or with C adsorption (right).