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Thermodynamics of catalytic nanoparticle morphology MICHAEL ZWOLAK, RENU SHARMA, PIN ANN LIN, Center for Nanoscale Science and Technology, National Institute of Standards and Technology — Metallic nanoparticles are an important class of industrial catalysts. The variability of their properties and the environment in which they act, from their chemical nature & surface modification to their dispersion and support, allows their performance to be optimized for many chemical processes useful in, e.g., energy applications and other areas. Their large surface area to volume ratio, as well as varying sizes and faceting, in particular, makes them an efficient source for catalytically active sites. These characteristics of nanoparticles – i.e., their morphology – can often display intriguing behavior as a catalytic process progresses. We develop a thermodynamic model of nanoparticle morphology, one that captures the competition of surface energy with other interactions, to predict structural changes during catalytic processes. Comparing the model to environmental transmission electron microscope images of nickel nanoparticles during carbon nanotube (and other product) growth demonstrates that nickel deformation in response to the nanotube growth is due to a favorable interaction with carbon. Moreover, this deformation is halted due to insufficient volume of the particles. We will discuss the factors that influence morphology and also how the model can be used to extract interaction strengths from experimental observations.

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