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Exploiting Automatic Image Processing and In-situ Transmission Electron Microscopy to Understand the Stability of Supported Nanoparticles

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The activity and lifetime of heterogeneous catalysts are intimately linked with their structural stability in reactive environments. However, it can be challenging to understand and predict how reactive environments lead to nanoparticle coarsening via center of mass motion and Ostwald ripening and how evaporation can lead to mass loss.

In this work, we develop and exploit advanced data analysis tools to track the temporal evolution of nanoparticles as a function of time, temperature, and reactive environment using transmission electron microscopy. The first portion of the talk will describe our development of a fast and highly accurate image segmentation approach based on deep learning. We describe how a systematic investigation of dataset preparation, neural network architecture, and accuracy evaluation lead to a tool for determining the size and shape of nanoparticles in high pixel resolution TEM images. [1]

In the second half of the talk, we will show how we exploit this approach to generate rich data regarding the complexities of nanoparticle coarsening, ripening, and evaporation. Au nanoparticles created through colloidal synthesis approaches undergo a combination of both evaporation and diffusive mass transport. We have developed an analytical model that describes this process and shows how local and long-range particle interactions through diffusive transport affect the evaporation process. The extensive data of the evolution of several hundred particles allows us to determine physically reasonable values for the model parameters, quantify the particle size at which Gibbs-Thompson pressure accelerates the evaporation process, and explore how individual particle interactions deviate from the mean-field model. [2]

Finally, during the evaporation process, we see strong evidence of the formation of specific facets as the particles shrink. We have used kinetic Monte Carlo methods and Density Functional Theory to investigate the atomistic processes in detail, and show a correlation between evaporation the formation of {311} facets and the evaporation process [3].

References:

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