Exploiting automatic image processing 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 both 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 will describe how a systematic investigation of dataset preparation, neural network architecture, and accuracy evaluation can lead to a generalizable tool for determining the size and shape of nanoparticles in high pixel resolution bright-field TEM images.[1]. In the second half of the talk, we will show how we exploit this analysis approach to generate rich data regarding the complexities of nanoparticle coarsening, ripening, and evaporation. In particular, we show how Au nanoparticles created through colloidal synthesis approaches [2] undergo a combination of both evaporation and diffusive mass transport. We have developed an analytical model that describes this process and shows how both local and long-range particle interactions through diffusive transport affect the evaporation process. The extensive data of the time evolution of several hundred particles allows us to determine physically reasonable values for the model parameters, quantify the particle size at which the Gibbs-Thompson pressure accelerates the evaporation process, and explore how individual particle interactions deviate from the mean-field model. [3] Recent extension of the approach to evaporated Au nanoparticles and Pt particles in reactive environments will be described.

References:

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