東京大学大学院工学系研究科 総合研究機構
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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 linked with their structural stability in reactive environments. We have developed and exploited machine learning methods to track the temporal evolution of Au nanoparticles deposited on SiN as a model system to understand this process. 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. We use this algorithm to generate data regarding the complexities of nanoparticle coarsening, ripening, and sublimation. We have developed an analytical model that describes this process, showing how local and long-range particle interactions through diffusive transport affect sublimation. The extensive data allows us to determine physically reasonable values for the model parameters, quantify the particle size at which Gibbs-Thompson pressure accelerates the sublimation process, and explore how individual particle interactions deviate from mean-field behavior. We observe that sublimation proceeds by sequential facet/defacetting transitions and utilize Kinetic Monte Carlo and Density Functional Theory to show how mobile adatoms form through desorption from low-coordination facets and subsequently sublimate. These results help to rationalize why evaporation rates vary between particles in a system of nearly identical nanoparticles. Recent work has extended this beyond the model case of Au to investigate Pt nanoparticles, which find ubiquitous use in heterogeneous catalysis. We'll describe how the reactivity of Pt with the Si substrate leads to silicide formation, which has very strong effects on the evolution of Pt nanoparticles. In particular, we show that changes in interfacial energy between the newly formed Pt_3Si and the underlying silicon drive particle motion, leading to particle coarsening.