The properties of ultra-thin metallic films are heavily dependent on the transition from discontinuous islands to continuous films. Additionally, devices assembled from nano-crystallite building blocks are also beginning to show promise for implementing novel applications. In some applications, the nanoclusters must remain isolated from one another, while in other applications, selective electrical contact is required. This research project focuses on the bonding and boundary formation process when nanoclusters are placed in contact with one another. This process is analogous to island impingement during thin film formation. The high surface curvatures of the islands provide a very strong driving force for bonding. An increase in strain energy is compensated by the reduction in surface energy. The intrinsic tensile stress generated by this process is measurable and expected to affect the thin film device properties.

The boundary formation process is being investigated primarily through the use of computer models. These computer models incorporate semi-empirical inter-atomic potentials and molecular dynamics to evolve a system of clusters in time. Through these calculations, we find that the times required for nanometer sized islands to form boundaries can be on the order of nanoseconds (see Figure 1) and that the boundary areas are consistent with predictions from continuum theory. Based on these findings, we are also implementing a finite element model, which incorporates the orientation and contact angle dependencies seen in the atomistic calculations.

In connection with the computational studies, we are using transmission electron microscopy (TEM) to investigate the coalescence and sintering behavior of model systems generated from colloidal suspensions and from pre-coalescence metallic thin films (see Figure 2). Defect structures observed in the TEM will be directly compared to computationally generated defects.

Figure 1: Distance between centers of mass evolution over time showing the completion of the boundary formation process in approximately 2 ns.

Figure 2: A nanoparticle array before (left) and after (right) heat treatment to induce particle sintering. The scalebars are 10 nm.