Understanding tungsten migration blazes trail for nano electronic device development

September 15 2011

Trios of tungsten atoms are greatly influenced in their migration across the wilds of a tiny particle by the shape of the particle, according to a team of experts, including Pacific Northwest National Laboratory's Dr. Fei Gao. The U.S. and China team performed complex computational simulations to determine the energetics involved in the tungsten cluster migration. They found that the 3 to 4 adatom, or surface atom, clusters prefer to form close-packed islands. The reorientation is the dominant migration mechanism for the dimer, while the net migration of lager clusters can be accomplished by the dimer shearing, concerted motion and rotation mechanisms.

The research was highlighted on the cover of the European Physical Journal B in March 2011 along with the peer-reviewed article: "Tungsten Clusters Migration on Nanoparticles: A Dimer Method Study."

The demand for miniaturization of electronic devices will benefit from a more in-depth understanding of nanostructured materials. Tungsten has unique properties such as high density, hardness, melting temperature, elasticity and conductivity, along with low thermal expansion. These unique properties and nanometer-sized particles can be used to store and arrange electrons for use by semiconductors, providing engineers with a material of lower resistance and improved conductivity.

Using supercomputers in the Environmental Molecular Sciences Laboratory, the research team performed the calculations necessary to search for possible transition states and migration paths for tungsten

clusters on tungsten nanoparticles, and corresponding migration energies for the possible migration paths of these clusters.

Tungsten clusters with up to four adatoms are found to prefer 2D-compact structures with relatively low binding energies. The team determined that the effect of interface and vertex regions on the migration behavior of the clusters is significantly strong compared to the nanoparticle size.

Migration mechanisms are very different when the clusters are located at the center of the nanoparticle and near the interface or vertex areas. Near the interfaces and vertex areas the substrate atoms tend to participate in the migration processes of the clusters, and can join the adatoms to form a larger cluster or lead to the dissociation of a cluster via the exchange mechanism, which results in the adatom crossing the facets.

The calculated energy barriers for the trimers suggest that the concerted migration is more probable than the successive jumping of a single adatom in the clusters.

The multi-scale computational method, ranging from ab initio calculation to long time dynamics method, will be further employed to study structural evolution of nanometer-sized metal clusters with increasing size and phase transformation of these metal clusters. These studies will provide significant insights into nanoscale catalysts, sensors and electrochromic applications such as smart glass where light or heat transmission properties of the glass are changed by applying voltage.

More information: Chen D, et al. 2011. "Tungsten Cluster Migration on Nanoparticles: Minimum Energy Pathway and Migration Mechanism." *The European Physical Journal B* 80(1):31-40.

Provided by Pacific Northwest National Laboratory