Low Energy Electron Enhanced Etching: Simulating Processes Involving Highly Excited and Unstable Systems

Hatem H. Helal, Markus J. Buehler, Julius Su, and William A. Goddard III  
*Materials and Process Simulation Center, California Institute of Technology*

H. Pat Gillis  
*Department of Materials Science and Engineering, UCLA and Systine Inc.*

The standard methods of quantum mechanics (QM) work quite well for describing both the ground electronic state structure and the reactions involving these ground states. However, there is little understanding of the dynamical processes of highly excited states or of what decompositions might result from various excitations. We are particularly interested in understanding the complex electronic rearrangements that occur during low energy electron enhanced etching (LE4). LE4 is a novel etching technique that avoids the surface damage inherent in traditional ion based etching processes. Our work focuses on applying QM methods to study the highly excited states created from electron impact and how these states lead to fragmentation. Previous models developed for electron stimulated desorption have shown that the system evolves into a localized two-hole state. Our simulations have found that a localized two-hole state will lead to a repulsive potential between the atoms involved in the localized holes. We have developed an algorithm to follow the dynamics of a molecular system after the creation of an excited state. These calculations were carried out within the newly developed Computational Materials Design Facility (CMDF).