

4. Reaction Dynamics at Semiconductor Surfaces

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The mechanism of the reactions of a gaseous species such as F_2 with a semiconductor surface such as Si is complex. The mechanism may involve several processes, including the adsorption of the molecule on the semiconductor surface, dissociation of the adsorbed molecule, diffusion of the dissociated species to a reactive site, reaction with the surface, and then desorption of the product molecule. The purpose of this research is to study the dynamics of the first two processes, the adsorption and dissociation of a molecule incident on a surface. We would like to understand how a molecule falls apart on a surface. For example, does the molecule first adsorb and then diffuse to a reactive site and then dissociate or are the dissociation and adsorption processes concerted? What feature of the potential energy surface of the molecule–surface interaction dictates which dynamics occur? Variation of the energy of the incident molecule is a convenient probe of these dominant features of the interaction potential because the dynamics and hence the observed dissociation probability depend strongly on the incident energy relative to the interaction potential.

However, studies of the effect of the energy of the incident molecule on the dissociation probability are virtually nonexistent because most surface studies are undertaken after adsorption of ambient molecules. This implies that molecules strike the surface from all directions and with energies characterized by a 300 K Maxwell–Boltzmann distribution. We have just begun to design and build an apparatus to investigate the effect of the incident energy on the probability of dissociative adsorption. This apparatus employs molecular–beam techniques to define and control the energy of the incident molecule (up to 50 kcal/mole and 10 kcal/mole translational and internal excitations, respectively). The presence and amount of dissociation are detected sensitively ($\geq 0.1\%$ of a monolayer) by high–resolution electron–energy–loss spectroscopy, a vibrational spectroscopy. These fundamental studies on the effect of a molecule's incident energy on dissociative adsorption are important because of the unknown chemistry these "hot" neutral molecules carry out during the plasma etching of semiconductors, where translationally and internally excited molecules are produced by numerous collisions with fast ions and electrons. The long–range goal of this research is to provide far–reaching correlations between the observed dynamics and the potential energy surfaces on which molecule–surface reactions occur.

