Doctoral Research at Brown University
"Studies of the Si/SiO_2 Interfaces (hard/dry materials)"

Si/SiO_2 interfaces has been the subject of intense study for last 3-4 decades because of the relevance to the microelectronics industry and have been long recognized as critical for device operation, yet the structure and reaction mechanisms of the Si/SiO_2 interfaces remains largely a matter for conjecture. In recent years, poorly understood reactions occurring at this interface have impeded the development of reliable devices with oxide thickness of under 100 Å.

At Brown, as a part of doctoral research, I have undertaken a study of the structure and reactivity of the Si/SiO_2 interfaces. A central part of the research design has involved the creation of model interfaces derived from cluster molecules such as those shown below.

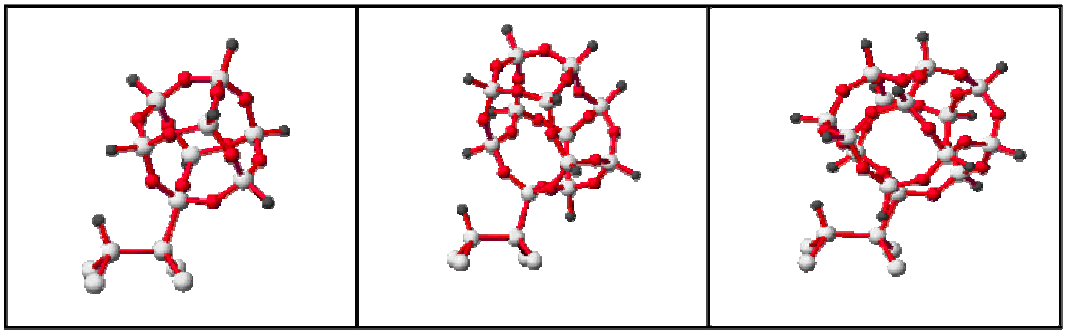

Figure 1. Appropriate cluster bound to a surface dimer by one vertex.
A hydrogen atom is also shown attached to the dimer.

We have characterized three model interfaces synthesized using the spherosiloxane clusters. These molecules, which simulate 3-4 layers of oxide, represent the first synthesis of silicon/silicon oxide interfaces of known structure. The primary characterization tool for both the model interfaces and the Si/SiO_2 interface has been synchrotron soft X-ray photoemission of Si 2p core-levels (Figure 2). Our new approach to Si 2p core-level shift assignments has profound implications for work concerning the structure of the silicon/silicon oxide interface. We have also applied the new shift assignments to explore the reaction of hydrogen atoms in the interface region. The development of model systems to aid in the complicated spectroscopic assignments of solid/solid interfaces is one important aspect of this work. These works have been published in the *Journal of the American Chemical Society* (116, 11819, 1994), *Applied Physics Letters* (68, 1081, 1996), *Phys.Rev.B*, (54, 7686, 1996), *J. Vac. Sci. Tech. B*, (14, 2824, 1996) and *Appl. Organometallic Chem.* (13, 279, 1999).

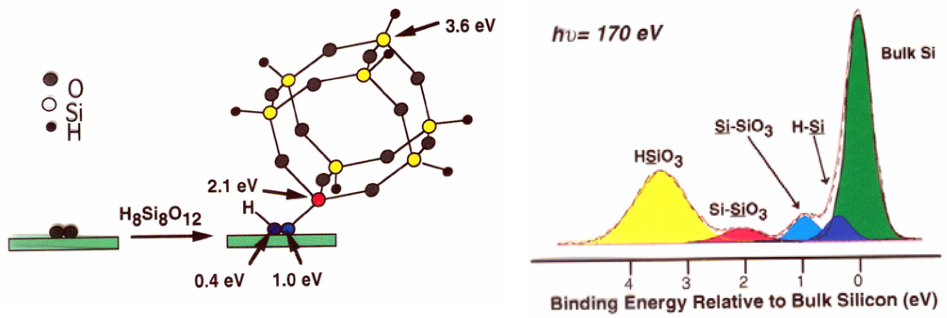

Figure 2. Characterization of the interface structure: Si 2p Core level Spectroscopy: The first opportunity to assign the binding energy shifts directly to known chemical moieties at Si/SiO_2 interface.