DYNAMICS OF HYDROGEN IN SILICON

Stefan K. Estreicher
Texas Tech University

Hydrogen is easily incorporated into crystalline silicon during a range of processing steps. It diffuses fast and binds covalently at native defects and impurities. These hydrogen-containing complexes are often stable up to several hundred degrees Celsius and their electrical and optical properties are very different from those of the original defect centers. The electrically active gap levels of defects and impurities shift upon hydrogenation, sometimes from the gap into a band (*passivation*), from a band into the gap (*activation*), or simply within the gap. New local vibrational modes (LVMs) are detected by FTIR or Raman spectroscopies, and photoluminescence band may appear or disappear. In Czochralski (oxygen-rich) Si, hydrogen enhances the diffusivity of interstitial oxygen in the 300-500°C temperature range. This results in enhanced O precipitation, which is of great importance to the gettering of transition metal impurities and processes involving native defects.

A substantial research effort on the part of experimentalists and first-principles theorists has resulted in the definite identification of many complexes containing hydrogen and native defects or impurities. However, many questions remain unanswered. For example, large concentrations of interstitial H_2 molecules in the bulk of Si can be achieved by high-temperature anneals a hydrogen gas or by exposure to a remote plasma at moderate temperatures. In both cases, the process begins with large concentrations of atomic hydrogen in the bulk. So far, molecular-dynamics simulations have failed to explain how the H_2 molecules form while another hydrogen dimer, H_2^*, never does. Other questions deal with the interactions between hydrogen and transition-metal impurities. The experimental information available to date on these complexes is mostly of electrical nature and theorists disagree on the interactions taking place and the structure(s) of the complexes. As for the H-enhanced diffusion of oxygen, several models have been proposed. But they are all incomplete and no experimental data are available. Another open question relates to the formation and growth of hydrogen 'platelets', large planar structures which are critical to the 'smart-cut' process.

In this talk, several of these issues are discussed from a theoretical (first-principles) perspective, with emphasis on unresolved problems. Constant-temperature molecular-dynamics simulations show the trapping of H at defects or impurities. Linear response theory allows the calculation of accurate dynamical matrices. Their eigenvalues give all the normal modes of the system (including the LVMs) and their eigenvectors show the relative motion of the atoms. The calculation of defect vibrational entropies is under way and should lead to the prediction of room-temperature free energies.