



# *Vibration Dynamics of Hydrogen and Oxygen Defects in Semiconductors*

**BAOZHOU SUN**

College of William & Mary, Department of Applied Science, 2005

Field: Interface and Surface Physics Degree: Ph.D.

Advisor: Gunter Luepke, Associate Professor of Applied Science

## Abstract

Characterization of defect and impurity reactions, dissociation, and migration in semiconductors requires a detailed understanding of the rates and pathways of vibrational energy flow, of the energy transfer channels, and of the coupling mechanisms between local modes and the phonon bath of the host material. Information on the inelastic microscopic interaction can be obtained by measuring the lifetime of local vibrational modes. This dissertation presents vibrational lifetime measurements of hydrogen and oxygen defects in semiconductors by means of time-resolved infrared (IR) pump-probe spectroscopy. In these experiments, a picosecond IR pulse excites a vibration of a significant fraction of point defects in a sample. This excitation causes a transient decrease in the absorbance of the sample, as there are fewer defects in the vibrational ground state that can absorb. The transmittance change is measured with a weaker probe pulse that passes through the sample after a variable delay, so that the evolution of the excited vibration can be followed in time. This technique enables the direct time-domain measurement of the lifetime of local vibrational modes.

First, we measured the vibrational lifetime of H- and D-related bending modes in Si and other semiconductors. Time-resolved pump-probe and linewidth measurements reveal that the lifetime of bending modes can be explained by an energy gap law, i.e., the decay time increases exponentially with increasing decay order.

Second, we present the vibrational lifetime measurements of a selection of Si-H stretch modes in crystalline Si. The lifetimes of interstitial-type defects are found to be a few picoseconds, whereas vacancy-type defects have lifetimes up to 300 picoseconds. The strong dependence of lifetime on the atomic structure of the defect suggests that pseudolocalized modes are involved in the vibrational relaxation of the stretch modes of hydrogen defects in Si. It is found that the energy relaxation of Si-H stretch modes does not decay by lowest order, i.e., low frequency modes are involved in the decay process.

Furthermore, we performed lifetime measurements of interstitial oxygen in Si and Ge. The lifetime of  $^{17}\text{O}_i$  in Si is half of  $^{16}\text{O}_i$  and  $^{18}\text{O}_i$ . A calculation of the three-phonon density of states shows that  $^{17}\text{O}_i$  lies in the highest phonon density resulting in the shortest lifetime. The lifetime of the  $^{16}\text{O}_i$  mode in Ge is measured to be 10 times longer than in Si. The interaction between the local modes and the lattice vibrations is discussed according to the activity of phonon combination.

These studies elucidate the dynamics of energy dissipation and vibrational decay channels of point defects in semiconductors. They provide a better understanding of the dissociation of Si-H and Si-O bonds and the strong hydrogen and deuterium isotope effect found in H-passivated semiconductor devices. The experimental results provide an indispensable benchmark for future theoretical investigations.