Vibrational Lifetimes of Hydrogen in Silicon

B. Sun and G. Lüpke,

Department of Applied Science, College of William & Mary, Williamsburg, VA 23187

N. H. Tolk and L. C. Feldman

Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235

Vibrational lifetimes of hydrogen- and deuterium-related stretch modes in crystalline silicon are measured by high-resolution infrared absorption spectroscopy and pump-probe transient bleaching technique using the Jefferson Lab. Free-Electron Laser (FEL). The lifetimes are found to be extremely dependent on the defect structure, ranging from 2 to 295 ps. Against conventional wisdom, we find that lifetimes of Si-D modes typically are longer than for the corresponding Si-H modes. Vibrational lifetimes have been obtained in the temperature range from 5 K to room temperature for the Si-H stretch modes of the H_2^* and $HV-VH_{(110)}$ defects in crystalline Si. The 2062-cm⁻¹ mode of the interstitial-type defect H₂^{*} has a short lifetime, $T_1 = 4.2$ ps at 5 K, whereas the lifetime of the 2072.5-cm⁻¹ mode of the vacancy-type complex HV·VH₍₁₁₀₎ is two orders of magnitude longer, $T_1 = 295$ ps. The temperature dependencies of the lifetimes of the two defects are found also to be extremely different, showing that the two modes have different decay channels. The 2062-cm⁻¹ mode of H_2^* decays into vibrational modes of 165 cm⁻¹, which are likely to be TA phonons. In contrast, the 2072.5-cm⁻¹ mode appears to decay into LA phonon modes of 343 cm⁻¹. Our results show that the multi-phonon coupling strengths depend strongly on the structure of the defect, i.e. highly distorted interstitial-type defects have larger coupling constants and couple to lower frequency modes than vacancy-type defects. The potential implications of the results on the physics of electronic device degradation are discussed.