Structural Characterization of Optically Active Defects in Selenium-Doped Silicon

BONNA NEWMAN, JOSEPH SULLIVAN, Massachusetts Institute of Technology, MARK WINKLER, MENG-JU SHER, Harvard University, MATTHEW MARCUS, SIRINE FAKRA, Lawrence Berkeley National Laboratory, ERIC MAZUR, Harvard University, TONIO BUONASSISI, Massachusetts Institute of Technology — We demonstrate that enhanced sub-bandgap absorption in ultra-doped Si is directly related to the chemical structure of the dopant atoms. Femtosecond-laser irradiation of a crystalline-Si wafer coated with a thin Se film results in doping concentrations of 1 at. % Se in a layer extending 200 nm from the surface. This layer absorbs over 90% of incident photons at wavelengths between 400 and 2500 nm, demonstrating the potential to increase the efficiency of Si-based solar cells. Se K-edge extended X-ray absorption fine structure (EXAFS) spectroscopy on infrared-absorbing samples reveals clusters of two or more dopant Se atoms. Thermal annealing results in a decrease in infrared absorption and an evolution of Se atom chemical state to isolated interstitial point defects. These results indicate that a Se complex is responsible for enhanced optical absorption and suggest a method to alter the absorption coefficient of silicon.