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Spectroscopic SHG and spectroscopic ellipsometry study of silicon nanocrystals embedded in SiO₂ JUNWEI WEI, ADRIAN WIRTH, MICHAEL DOWNER, University of Texas at Austin, Department of Physics — The light-emitting silicon nanocrystals (Si NCs) embedded in silica matrix open up the possibility for silicon photonics. Optical spectroscopy can help elucidate unique, but poorly understood, bonding structures at the nano-interfaces that are responsible for the efficient photoluminescence. Here we present SHG amplitude and phase spectra of a 1 μ m-thick layer of 3 nm \pm 30% diameter Si NCs prepared by implanting Si ions into SiO₂ then annealing in Ar or H₂/Ar mixture at 1100°C using cross-polarized two-beam second-harmonic generation (XP2-SHG). We also measure the linear dielectric function of the NC layer using spectroscopic ellipsometry (SE). The linear spectra show a significant reduction in the dielectric functions in Si NCs compared to bulk silicon. The pronounced E₂ critical point transition peak is somewhat blueshifted to the bulk E₂ peak while E₁ transition is strongly suppressed. The SHG spectra are only slightly perturbed by annealing in hydrogen. A fit of the SHG amplitude and phase spectra using model resonance functions yields resonances different from the linear spectra. A model with an intermediate transition layer of variable composition between the Si NC core and the amorphous SiO₂ matrix is introduced to explain the linear and SHG spectra.

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