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Optical Absorption in Small Diameter Si Nanowires KOFI ADU, GUGANG CHEN, HUMBERTO GUTIÉRREZ, PETER EKLUND, Department of Physics, Pennsylvania State University, University Park, PA 16802, U.S.A — Optical absorption spectra on 3 sets of Si nanowires with most probable diameter 3.5 nm, 5.5 nm and 9 nm are presented. In the optical absorption, apart from the direct gap absorption at $E_{\Gamma 1} \sim 3.4$ eV and $E_{\Gamma 2} \sim 4.2$ eV, we observed two additional strong absorption bands near 1.5 eV and ∼2.5 eV. Interestingly, these lower energy features are not expected on the basis of the bulk dielectric function of Si. They are observed experimentally to increase in intensity with decreasing nanowire diameter. It is also interesting that the 1.5eV peak does not shift with decreasing wire diameter. This behavior leads us to tentatively assign this structure to SiO2:Si interface states. On the other hand, the ∼2.5 eV absorption band exhibits a systematic blue shift with decreasing diameter. Many of the features in the experimental absorption spectrum will be explained on the basis of dielectric function calculations carried out in the discrete dipole approximation (DDA). The DDA model results are shown to depend on the nanowire diameter/length and the thickness of amorphous SiO2 shell.

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