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Tuning of Refractive index and Optical Band Gap in Oxidized Silicon Quantum Dot Solids

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Quantum dots (QDs) or nanocrystalline semiconductors whose radii are less than tens nanometers have discrete energy levels resulted from the confinement of carriers in all three spatial dimensions, known as quantum confinement effect. Different from well-investigated II-VI QDs containing cadmium, silicon QDs (Si QDs) are nontoxic, cheap, and relatively easy to integrate into industrially well-established silicon process. On the other hand, what kind of collective properties arise when the semiconductor quantum dots (QDs) are assembled into two or three dimensional arrays has drawn much interest. The term of "quantum dot solids" is used to indicate three dimensional assemblies of the semiconductor QDs. The quantum dot solids with controlled and variable electron densities have been expected to be quite useful in the field of opto-electronic switches, LEDs, Lasers, and solar cells. In this work, we originally intended to fabricate the Si QD solids from pure *n*-butyl capped Si QDs by spin-coating but, unfortunately, the Si QDs had been oxidized either in its synthetic process or storage period in diethyl ether solvent prior to film fabrication. So we changed the direction of research to investigate the variation of Si QD solids' optical and electrical properties as oxidized. Oxidation of the Si QD solids was confirmed by the chemical composition obtained from FT-IR and XPS. Refractive index values and thicknesses of the Si QD solids obtained from SE were decreased as oxidized, due to increase of SiO₂ phase, decrease of Si phase, and decomposition of butyl groups capping the Si QDs respectively. Using UV absorption peaks of the Si QD solids, the diameters of the Si QD solids were roughly estimated to 0.8~0.7 nm. PL properties of the Si QD solids were also investigated. And it was suggested that the origin of the Si QD solids' PL properties is the Si=O bond at the Si/SiO₂ interface in the oxidized Si QD. In addition, the variation of the Si QD solids' dielectric constants according to oxidation of the Si QD solids was investigated by measuring C-V curves which were measured on metal-insulator-semiconductor (MIS) structure.