Study of Si nanocrystals embedded in SiO2 matrix using Raman spectroscopy/mapping

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Nanostructures show unique properties due to their large surface-to-volume ratio and or quantum size effects. To have desired control on the growth of a nanocomposite (nanostructures embedded into a processable matrix), it is imperative to understand the characteristic of individual component in the presence of other and the formation mechanism(s) of nanocomposites. Raman spectroscopy/mapping being an excellent non-contact, non-destructive optical tool can effectively be used to probe spatial variation of local bonding environment in nanocomposites. The motivation of this work is to discuss the application of Raman spectroscopy/mapping for the investigation of Si-SiO2 nanocomposites.

In Si-SiO2 nanocomposites grown by pulsed laser deposition, large variation (495 - 519 cm-1) in Si phonon frequencies was found to arise from surface/interface and core of Si nanocrystals. Raman spectroscopy/mapping study showed that the extended interface generated due to the interaction between surface atoms of Si nanocrystal and Oxygen in the matrix plays an important role in the Raman spectra, contribution of which depends on the size of a Si nanocrystal. Further, it was observed that resonance Raman scattering is crucial for the observance of these surface/interface phonons. XPS measurements showed observance of Si1+ and Si3+ suboxide states with higher intensity in the nanocomposites corresponding to higher content of core and surface/interface and phonons in Raman mapping, respectively. Observed one to one corroboration between Raman mapping and XPS was understood as due to formation of smaller Si nanocrystals in Si excess SiO2 (top layer) during annealing at 800 oC. The understanding developed can conclude the ongoing debate on large variation in Si phonon frequencies in Si–SiO2 nanocomposites reported in the literature.

In short, Raman spectroscopy/mapping showed that interaction between semiconductor nanocrystal and matrix plays an important role in determining the morphology and properties of nanocomposites.