Nanocomposites and nanomaterials

Raman study of reversible photo-induced cubic-hexagonal transformation of nanocrystalline silicon

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Silicon nanocrystals (NCs) have shown great potential in a range of applications. Like other semiconductor materials, when Si crystallites are made smaller than the exciton Bohr radius, their electronic and light emission properties can be tuned via size-dependent quantum confinement and further modified by surface chemistry. Usually Si crystallizes in the cubic diamond structure. However, several other Si polytypes are known, which are stable in bulk only at high pressures , but can be stabilized at ambient pressure in Si nanowires. Among these polytypes, hexagonal Si (h-Si) is the most often reported one and promising for novel optoelectronic applications due to its linear and non-linear optical properties.

Two kinds of Si samples were studied. Sample 1 was obtained by grinding of silicon plates in a ball mill resulting in a rather quasi-continuous distribution of crystallite sizes in the nano- and micrometer range. Sample 2 was commercially available "NanoAmor" Si NCs with an average size of 100 nm.

A photoinduced cubic-to-hexagonal phase transition in Si nanocrystals is studied by Raman and photoluminescence (PL) spectroscopies. The structural transformation is observed in Raman/PL spectra *in situ* by increasing the power density of the exciting laser beam. The formation of the hexagonal structure is concluded based on the simultaneous appearance of characteristic Raman peaks near 500 cm^{-1} and intense PL with spectral positions reported previously for hexagonal Si. The high PL intensity indicates that the new phase formed has a direct bandgap and the spectral position of the PL band is in good agreement with that reported previously for h-Si. The phase transition occurs due to heating of the nanocrystals by the laser beam, but it is supposed to be a photo-induced effect, as it does not occur as a consequence of solely thermal heating. Both the structural transition and concomitant switching of the bright PL emission are reversible and are supposed to be of interest from the viewpoint of application.