Indian Journal of Engineering & Materials Sciences Vol. 16, June 2009, pp. 188-192

Synthesis and optical properties of CdTe nanocrystals with improved optical properties

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Received 24 February 2009; 29 April 2009

CdTe nanocrystals are prepared by hydrothermal route using the reaction between Cd^{2+} and KHTe in the presence of thioglycolic acid as the stabilizing agent. Hydrothermal synthesis under optimum conditions resulted in a rapid growth. CdTe nanocrystals with high PL intensity and narrow PL spectra are obtained in less time. The growth mechanism of CdTe nanocrystals is investigated. The growth rate in the initial stage of synthesis is higher in hydrothermal synthesis resulting in an increased growth in diffusion controlled focused region.

Keywords: CdTe, Nanostructures, Hydrothermal, Luminescence

CdTe is a semiconductor material with band gap energy of 1.56 eV and found application in different research areas ranging from microelectronics to fluorescent biolabeling. This is due to the great tunability of its electrooptical properties, which is achieved by size, surface, and morphological control of the particles in the quantum confinement regime¹⁻³. The investigation and optimization of semiconductor nanoparticles synthesis is an important problem. Photoluminescence (PL) quantum efficiency near to 65% is achieved at room temperature in CdTe nanocrystals (NCs) synthesized by metal-organic technologies⁴. Water based routes offer advantages due to simplicity, use of nontoxic solvents and low reaction temperatures, stability of PL properties and the possibility of NC size tunability⁵⁻²⁰. Moreover, small sized nanocrystals are possible. The width of emission peaks is somewhat narrower than that of the nano-crystals produced by other routes. Effective passivation by the formation of cadmium thiol complexes at the surface was found to be the origin of high PL quantum efficiency¹¹. The thiol capped CdTe were reported to yield Quantum yield as high as 80%¹². Aqueous CdTe NCs have been successfully synthesized by using refluxing^{5,6} hydrothermally (in an autoclave)⁷ as well as a microwave irradiated vessel^{8,9}. Hydrothermal synthesis is a low cost synthesis route and highly crystalline product with narrow grain size distribution and high purity without post heat treatment could be obtained. The PL can be tuned in a wide spectral range using hydrothermal synthesis¹¹⁻¹⁶.

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In the present work, the optical properties of hydrothermally synthesized CdTe nanocrystals prepared by aqueous route were investigated. The associated change in size, emission peak position, intensity with increasing reaction time and temperature were studied Effect of increasing the hydrothermal synthesis temperature and time resulted in luminescence peak shift, which can be correlated to particles growth. Further, the growth kinetics of CdTe nanocrystals was investigated in thiol stabilized aqueous medium under different experimental conditions.

Experimental Procedure

The thiol capped CdTe NCs were prepared by the hydrothermal route at different temperatures. First KHTe was generated from the reaction of Te powder with KBH₄ in the presence of N₂ gas. Precursor solution of CdTe nanocrystals was prepared by adding KHTe solution to (CH₃COO)₂.2H₂O and thioglycolic acid in the presence of N₂. The molar ratio of Cd: Te: thiol was fixed at 4:1:5. The concentration of the precursor solution was kept as Cd = 2 mmol, pH value was fixed at 11. The CdTe precursor solution was put into Teflon lined stainless steel Autoclave. Different particle sizes were obtained by heating at 120°C, 140°C and 170°C for different duration. Another batch of CdTe nanoparticles was similarly prepared by refluxing the precursor solution for different duration at 100°C. TEM was conducted on a JEM200 CX transmission electron microscope to observe the microstructure of the samples. For TEM observations, a drop of as synthesized colloidal solution was placed on carbon coated copper

grids and allowed to dry. UV-vis optical absorption was measured by means of a Shimadzu UV-vis spectrophotometer. Photoluminescence (PL) measurements have been performed at room temperature a using an argon ion laser system and a Bentham monochromater system.

Results and Discussion

Refluxing at 100°C

Figure 1 (a,b) shows the absorption and luminescence spectra of the as prepared colloidal CdTe NCs grown for different reflux (100°C) period. On prolonging the refluxing time, the growth of the CdTe NCs was clearly evident by the shift of both absorption and emission spectra to longer wavelength. The emission peak shifted to 610 nm on refluxing for 20 h.

The luminescence intensity of as prepared sample was low but on increase in reflux time the luminescence intensity increases. High PL intensity and narrow emission width indicates growth of NCs with few electronic defect sites. FWHM of about 35-45 nm obtained for these samples shows a rather narrow particle size distribution (\sim 10%).

Hydrothermal synthesis at different temperatures

Figure 2 (a,b) shows the absorption and emission spectra for CdTe NCs synthesized at different



Fig. 1- UV-Vis and PL emission spectra of CdTe NCs synthesized at 100°C



Fig. 2— Absorption and emission spectra of CdTe NCs prepared at different temperatures