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Effect of Cu doping on Structural and Optical properties of CdS Nanoparticles

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Abstract: Undoped and Cu doped CdS nanoparticles were synthesized in aqueous solution by chemical co-precipitation method using EDTA as a capping agent. As synthesized samples were characterized by X-ray diffraction (XRD), energy dispersive analysis of X-rays (EDAX), diffuse reflectance spectra (DRS). X-ray diffraction (XRD) analysis reveals that undoped CdS nanoparticles are in cubic phase, where as Cu doped CdS nanoparticles are in mixed phase of cubic and hexagonal. EDAX spectra confirmed the presence of Cu in the samples with expected stoichiometric composition. DRS and corresponding Kubelka–Munk plots reveal that the band gap is narrowing with Cu doping.
Keywords: CdS: Cu, chemical synthesis, XRD and DRS.

1. Introduction and Experimental:

In recent years, semiconductor materials in nanocrystalline form and their synthesis, have gained huge interest due to their unique optical and magnetic properties. Cadmium sulfide nanomaterials are most widely studied binary chalcogenide material belonging to the II-VI group. CdS materials have been realized in the form of nanoparticles, nanowires, nanorods, nanobelts etc [1, 2]. However, due to the ease of preparation and versatile properties of nanoparticles most of the studies were focused on CdS nanoparticles. Magnetic elements such as Mn, Fe, Co, etc. were used as dopants to tailor the optical and magnetic properties of CdS nanostructures [3]. Here, in the present investigation we present the influence of Cu dopant concentration on the crystal structure and the optical properties of CdS: Cu nanoparticles synthesized by chemical co-precipitation method. Although many researchers have synthesized CdS: Cu nanoparticles, yet there is large scope in studying the doping effect on the optical properties of this material [4,5]. The effects of external and internal doping in the properties of material as well as the physics of doping pattern are yet to be understood. Hence more experimental findings are desirable for modulating future device oriented optical properties.

$Cd_{1-x}Cu_xS$(x=0.00, 0.01, 0.02, 0.03, 0.04 and 0.05) nanoparticles were prepared by chemical co-precipitation method with EDTA as a surfactant. The reactants used in present wok were (Cd $(CH_3COO)_2$ $.2H_2O$), $CuCl2.6H_2O$, Na_2S and EDTA(Ethylene diamine tetra acetic acid). All the chemicals were of analytical grade and were used without further purification. Doubled distilled de ionized water was used as the reaction medium in all the synthesis steps. In a typical synthesis 0.2M of (Cd $(CH_3COO)_2.2H_2O$) and $CuCl_2.6H_2O$ (at%

in Cu, x=0.01,0.02,0.03,0.04 and 0.05) each in 50 ml deionised water were dissolved. Subsequently stirring for 30 min, Na_2S (50 ml) solution was added drop wise to the above mixture under continuous stirring for 8hr at room temperature till a fine precipitate was formed. When the reaction was completed, the products were collected and washed thoroughly with a distilled water, and finally dried at 80^0 C for 3 hr for obtaining $Cd_{1-x}Cu_xS$(x=0.00, 0.01, 0.02, 0.03, 0.04 and 0.05) nanoparticles. Undoped CdS nanoparticles were also synthesized by the same procedure. The X-Ray diffraction patterns were obtained using seifert 3003TT X-ray diffractometer. Diffuse reflectance spectra of the samples were recorded at room temperature using Jasco V570 UV-Vis spectrophotometer in the wavelength range 400–800 nm.

2. Results and Discussion:

Elemental and Structural analysis:

Fig.1 shows EDAX spectra of $Cd_{1-x}Cu_xS$(x=0.03) nanoparticles. The EDAX spectra indicate the presence of Cd, S and Cu in the sample. Fig.2 shows the XRD Pattern of the undoped and doped nanoparticles. From the XRD pattern of the CdS, it is difficult to obtain the perfect crystal structure, because of the larger broadening and overlapping of cubic and wurtzite XRD patterns. Hence the undoped CdS can be considered as crystallized in cubic structure only. But in the Cu doped CdS nanoparticles the diffraction peaks positioned at 2θ values of 27.11^o,44.41^o,51.71^o and a small peak at 71^o were observed and they were indexed as (002), (220), (311) and (211) planes corresponding to that of a mixed state of zinc blende and wurtzite structure. The average size of the particles has been estimated using the Debye –Scherer formula, $D=0.89\lambda/\beta\cos\theta$, where λ is the wavelength of X-ray radiation, β is the full width at half maximum of the peak at diffraction angle θ. From the XRD studies the measured average crystallite size were in the range of 3.9-2.58 nm. The decrease of crystallite size with Cu doping may be due to the small ionic radii of Cu^{2+} (0.057 nm) when compared to Cd^{2+} ion (0.096 nm). Fig. 3 shows the room temperature diffuse reflectance spectra of the synthesized Cd_{1-x} Cu_xS (x=0.00, 0.01, 0.02, 0.03, 0.04 and 0.05) nanoparticles. The reflectance was increased after doping and it was dropped in the UV-region due to onset of fundamental absorption. However with increasing Cu content there is a marked decrease in reflectance in samples of higher dopant concentrations. This decrease may be due to light being scattered by grain boundaries as well as the Cu clusters which reflect the incident light. The characteristic absorption edge of the Cd_{1-x} Cu_x S (x=0.00, 0.01, 0.02, 0.03, 0.04 and 0.05) nanoparticles were in the range of 290 nm to 700 nm. The bandgap of the Cd_{1-x} Cu_x S (x=0.00, 0.01, 0.02, 0.03, 0.04 and 0.05) nanoparticles was estimated from the diffuse-reflectance spectra by plotting the square of the Kubelka–Munk function $F(R)^2$ versus energy and extrapolating the linear part of the curve to $F(R)^2 = 0$, The absorption edges are seen to be shifted towards higher wavelengths/lower energies (from 2.49 eV to 2.38 eV) with increasing Cu content as shown in Fig. 4. However the decrease in the bandgap with increasing the doping concentration due to sp-d exchange interaction between the band electrons and localized d electrons of the Cu^{2+} ions substituting Cd^{2+} ions. Although P.Reyes et al also reported similar decrease in the bandgap in Cu doped CdS nanopowders [5].

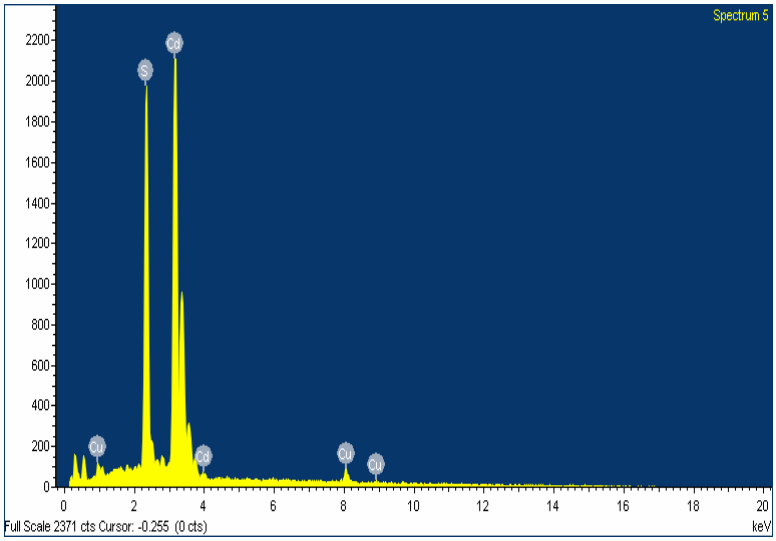

Fig.1 EDAX spectrum of 3% Cu doped CdS nanoparticles.

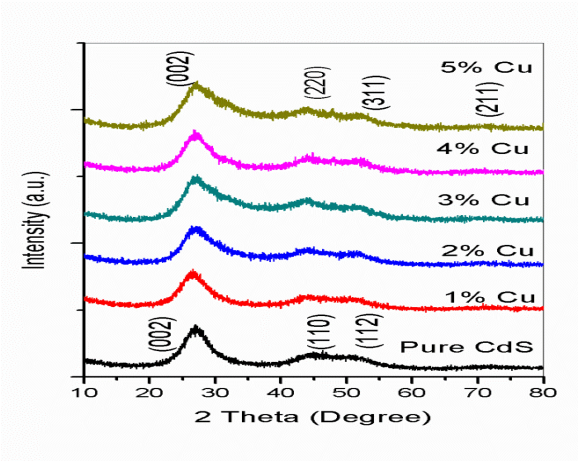

Fig.2 X-ray diffraction patterns of Cd_{1-x} Cu_x S (x=0.00, 0.01, 0.02, 0.03, 0.04 and 0.05) nanoparticles.

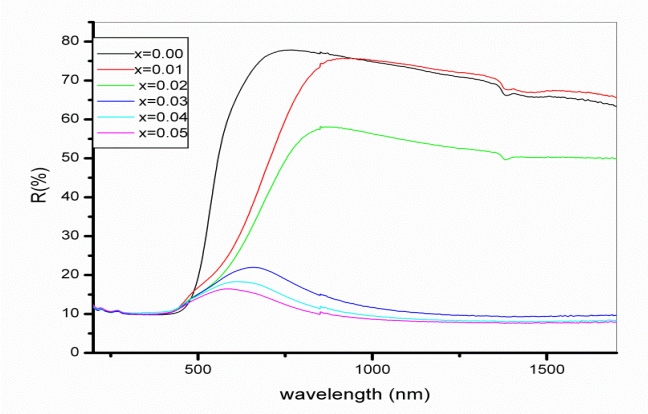

Fig.3 DRS of Cd_{1-x} Cu_x S (x=0.00, 0.01, 0.02, 0.03, 0.04 and 0.05) nanoparticles.

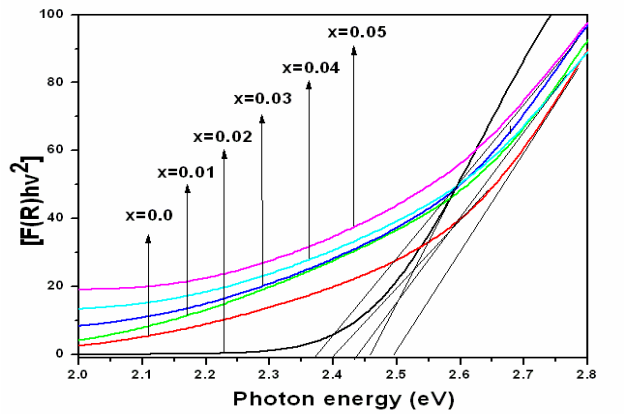

Fig.4 Kubelka-Munk plots and bandgap estimation of Cd_{1-x} Cu_x S (x=0.00, 0.01, 0.02, 0.03, 0.04 and 0.05) nanoparticles.

In summary pure CdS and Cu doped CdS nanoparticles have been prepared by chemical co-precipitation method with EDTA as a capping agent. The compositional analysis results show that Cd, Cu and S are present in the samples. The X-ray diffraction patterns show that the Pure and Cu doped CdS nanoparticles exhibit mixed state of zinc blende and wurtzite structure and the average particles size of nanoparticles is in the range of 3.9 nm to 2.58 nm. DRS spectra and corresponding Kubelka–Munk plots reveal that the bandgap is decreased with Cu doping showed that as the doping concentration increased the bandgap decreased.

3. References:

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