

Structure and optical characterization of nickel-doped nano CdS powder

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Nanocrystalline CdS:Ni²⁺ powder was synthesized in the laboratory at 280K using hydrothermal process without any capping agent. These Powders were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM). XRD patterns for Nickel doped and undoped CdS powders showed broad peaks corresponding to cubic CdS. The shift of the diffraction peak (111) towards higher angle is believed to result from the incorporation of Ni ions into the CdS lattice. Size of nanocrystallites was estimated to (~ 6 nm) using Scherrer's equation. SEM observations showed the presence of nanocrystallites forming spherical aggregates of around 50 to 60 nm in diameter. EDAX confirm the chemical composition of CdS: Ni²⁺.

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1. Introduction

Nanocrystalline dilute magnetic semiconductors show different properties in comparison to bulk and form a new class of materials which have potential applications in spintronics and photonic devices. Size dependence of optical properties [1-3] of nanocrystalline semiconductors makes them an interesting candidate for photonic applications. Semiconductors like CdS, CdSe and CdTe are well studied due to easy manifestation in optical properties as a function of size of nanocrystals. Several methods have been reported to make thin films and powders of nanocrystalline semiconductors [5,6,7]. In addition to physical routes, the preparation of metal chalcogenides thin films has been attempted by wet chemistry approaches like hydrothermal method. This technique is simple, inexpensive and works at low temperatures, which enables the use of practically any case.

Doped semiconductor nanocrystals (NCs) have attracted research interests in the recent years. These materials exhibit novel size dependent properties. Thus they are under active consideration as potential candidates in flat panel displays, optoelectronic devices, and so on. The properties such as optical absorption and luminescence are strongly modified in semiconductor nanoparticles due to size quantization. In a semiconductor nanoparticle, the size dependent properties appear when the radius of the particle is comparable to the Bohr radius of the exciton in the bulk material. In Particular II-VI semiconductor nanocrystals (NCs) have been of interest to the phosphor researchers [8, 9, 10]. Studies on the luminescence properties of alkaline earth sulphides with different activators have drawn considerable attention due to their potential use for electroluminescence and cathodoluminescence displays. In these materials, various defect sites in host, activator and charge compensator

doped in the host matrices can serve as emission centers and affect the luminescence of phosphors.

In this paper we reported to confirm of incorporation of Nickel ions into CdS in the terms of Structural and optical characterization.

2. Experimental details

2.1 Powder processing

Cadmium sulphide and nickel doped cadmium sulphide have been synthesized in the laboratory at low temperature (273K) using hydrothermal process. All the chemicals were of analytical grade and were used without any further purification. Appropriate amount of zinc nitrate cadmium nitrate tetrahydrate ($\text{Cd}(\text{NO}_3)_2 \cdot 4 \text{H}_2\text{O}$) were used as cadmium source along with sodium sulphide (Na_2S) as sulphur source. Nickel sulphate hexahydrate ($\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$) was used as nickel source. For CdS:Ni²⁺, Sodium sulphide and nickel solution is added to it drop wise separately with controlled drops in solution containing cadmium at 273K. Uniform magnetic stirring is provided for the better atomic diffusion during the length of the reaction. The resulting precipitates were filtered off and washed several times in distilled water. The precipitates were then dried in hot air oven at 50°C. Final products were then obtained by crushing dried precipitate using pestle mortar. In this paper we have reported the optical and structural result of pure CdS and Nickel doped CdS with the same process.

2.2 Characterization Detail

The crystal structure of CdS and CdS:Ni nano powders were characterized by X-ray diffraction (XRD)

using a Bruker D8 Advance diffractometer with $C_u K_\alpha$ target ($\lambda = 1.54056 \text{ \AA}$) radiation. The coherently diffracting domain size (d_{XRD}) was calculated from the integral width of the diffraction lines using the well known Scherrer equation, after background subtraction and correction for instrumental broadening [11]. The scan rate used was 1° min^{-1} and the scan range was from 20° to 60° . Microstructural and chemical analysis of the samples, were carried out by using field emission scanning electron microscope (FESEM - FEI Quanta 200) equipped with an Oxford Inca energy dispersive x-ray (EDX) detector. Optical absorption was measured in the 200–1300 nm wavelength range using UV-Vis-NIR spectrophotometer (Cary 5000 Varian).

3. Results and discussion

Crystal structure and average crystallite size of the powder products were investigated through XRD studies. Figures 1 shows the XRD patterns of the CdS and nickel doped CdS powders. Broad diffraction peaks in all the patterns were in well accordance with the characteristics of nano sized materials. It can be seen that all the samples exhibited a cubic structure, which was consistent with the previous result reporting that CdS exist in cubic structure at low temperature. However the diffraction peak (111) shifted to a higher angle to approach the pure NiS.

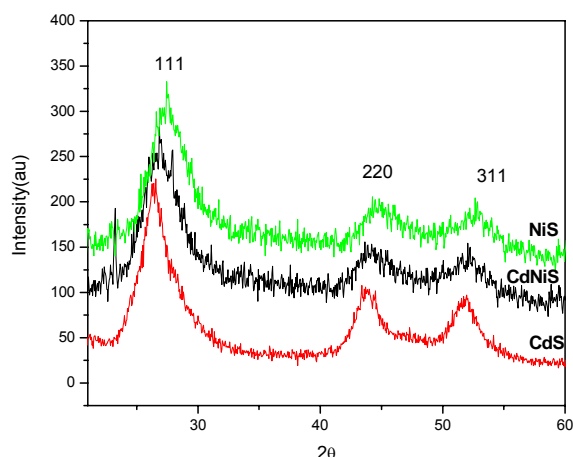


Fig. 1. X-ray diffraction pattern of CdS, Nickel doped CdS and NiS.

This shift towards higher angle is believed to result from the incorporation of Ni ions into the CdS lattice. In order to calculate the particle size, d_{XRD} of the samples we have used the Scherrer formula [12]

$$d = \frac{0.9\lambda}{B \cos \theta_B}$$

where λ , θ_B and B are the X-ray wavelength (1.54056 \AA), bragg diffraction angle and line width at half

maximum. The size of the CdS nano particle has been found 6nm which is a good estimate with the SEM result. Changing diffraction angles (2θ) as doping and the corresponding d -spacing of samples calculated according to the Bragg diffraction equation ($2d \sin \theta = \lambda$, where λ is 1.54056 \AA of $C_u K_\alpha$ radiation).

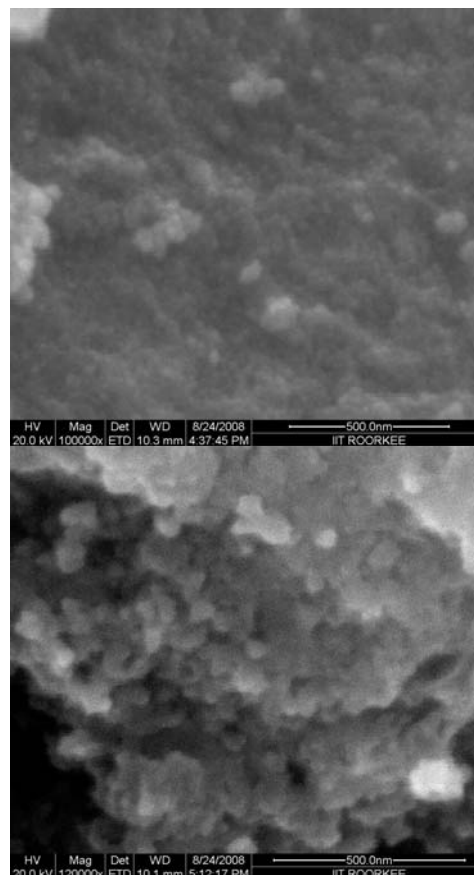


Fig. 2 (U) SEM micrograph of CdS and (L) SEM micrograph of Nickel doped CdS.

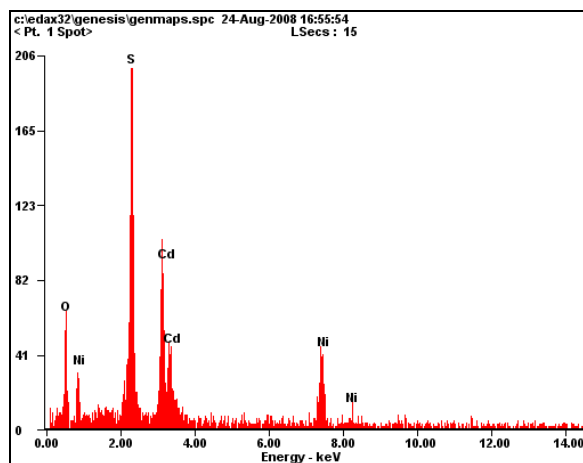


Fig. 3. EDX analysis of Nickel doped CdS

Microstructural and chemical analysis of the samples, were carried out by using field emission scanning electron microscope (FESEM - FEI Quanta 200) equipped with an Oxford Inca energy dispersive x-ray (EDX) detector. The Field emission scanning electron micrographs (FESEM) micrographs evidently show the microstructural heterogeneities. Figure 2 shows the shape and sizes of these particles were uniform. In these samples less compact agglomerates prismatic particles of 50-60 nm range were observed. A big difference has been seen in the morphology of CdS and Nickel doped CdS.

An EDX spectrum normally displays the peaks corresponding to the energy levels for which the most X-ray had been received. An EDX spectrum plot not only identifies the element corresponding to each of its peak, but the type of X-ray to which it corresponds as well. For example, a peak corresponding to the amount of energy possessed by X-rays emitted by an electron in the L-shell going down to the K-shell is identified as $K\alpha$ peak. The peak corresponding to X-rays emitted by M-shell electrons going to the K-shell is identified as $K\beta$ [13]. The EDX spectrum has shown in figure 3. However, the elemental compositional data can be obtained using EDX pattern. The results indicate that only Cadmium, Nickel and sulphur elements are present in the specimen.

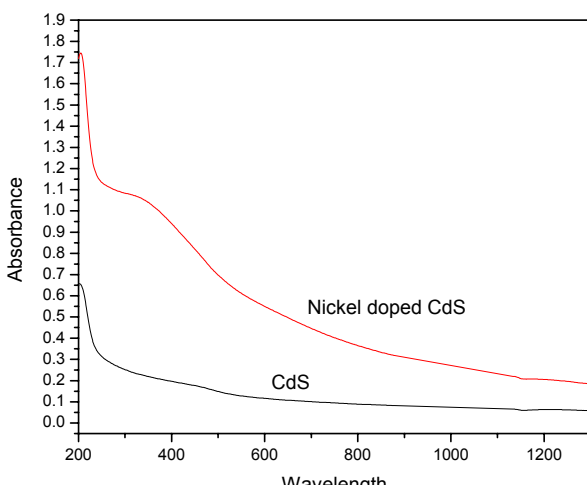


Fig. 4. Absorption spectra of CdS and nickel doped CdS nano powder.

Fig. 4 shows the absorption spectra of CdS and nickel doped CdS nano powders dispersed in deionized water. It is observed that the absorption coefficient of doped CdS is higher than pure CdS nanopowder and it has been clearly seen that red shift in the band edge on the doping of nickel in CdS confirm the incorporation of nickel in CdS lattice. The energy band gap is determined using absorption spectra with the help of Tauc relation [14]. Band gap of CdS nano powder is 2.89 eV has been shifted to 2.2 on the doping of nickel.

4. Conclusion

This work gives a conclusion that nickel can be incorporated with CdS using a very simple synthesis method (Hydrothermal). Structure and optical properties of the nickel doped CdS have been tailored. As nickel is a good ferroelectric material, we expect this may be an advantage to use as a dilute magnetic semiconductor for device application.

References

- [1] A. D. Yoffe, *Adv. Phys.* **42**, 173 (1993).
- [2] J. Nanda, K. S. Narayan, B. A. Kuruvilla, G. L. Murthy, D. D. Sarma, *Appl. Phys. Lett.* **72**, 1335 (1998).
- [3] Y. Kayanuma, *Phys. Rev. B* **38**, 9797 (1998).
- [4] Li-Yu Lin and Teng-Ming Chen *Tamkang Journal of Science and Engineering*, **5**, 187 (2002)
- [5] V. Ghiordanescu, M. Sima, M. N. Grecu, L. Mihut *J. Optoelectron. Adv. Mater.* **521** (2001)
- [6] S. Sirohi, T.P., Sharma *Optical Materials* **13**, 267 (1999)
- [7] P.P. Hankare, P.A. Chate, D.J. Sathe, M.R. Asabe, B.V. Jadhav, *Journal of Alloys and Compounds*, **474**, 347(2009)
- [8] I. Bank, *J. Optoelectron. Adv. Mater.* **11**, 91 (2009)
- [9] I. Banik, *J. Optoelectron. Adv. Mater.* **10**, 475 (2008).
- [10] Shikha Tiwari and Sanjay Tiwari, *Cryst. Res. Technol.* **41**, 78 (2006)
- [11] F. Boulch, M.-C. Schouler, P. Donnadieu, J.-M. Chaix, E. Djurado, *Image Anal Stereol* **20**, 157 (2001).
- [12] Cullity B.D., *Elements of X-ray Diffraction* Addison-Wesley Publication (1956)
- [13] S. Senthilkumar, K. Rajendran, S. Banerjee, T. K. Chini, V. Sengodan, *Mat. Sci. Semicond. Proc.* (2008),
- [14] J. Tauc (Ed.), *Amorphous and Liquid Semiconductor*, Plenum Press, New York, 1974, p. 159.

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