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OPTICAL AND LUMINISCENT PROPERTIES OF Ni^{2+}DOPED PVA CAPPED CdTe NANOPARTICLES

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ABSTRACT
Cadmium telluride is used for a variety of applications being a semiconductor material. Ni^{2+} doped PVA capped CdTe nanoparticles were prepared by co-precipitation method. Several spectroscopic techniques have been carried-out on to the prepared samples such as Optical, EPR, and Photoluminescence. The energy bandgap value is evaluated from optical studies.Optical absorption is due to vibrational bands of Nickel ion, $Ni^{2+}(d^8)$ which give rise to ^3F, ^3P, ^1D in the wavelength region 400-800 nm. The violet and blue emission bands in the visible region are obtained from the PL studies.
Keywords: CdTe, PVA, Co-precipitation, Ni^{2+} ions, optical, EPR and PL Studies.

INTRODUCTION

From the past few decades researchers have made an interest for the fabrication and development of semiconductor devices, nanomaterials like nanorods, nanowires, quantum dots nanotube, nanopowders etc[1]. '1D' nanocrystal semiconductors are having excellent physical properties such as structural, optical and electrical which is used in many applications such as modern electronic devices, sensors, and photonics materials. In general, there are several methods like solution cast technique, vapor phase approach, vapor liquid growth, co- precipitation method, sol-gel method , solution phase growth based on capping agents are used for the synthesis of nano- particles[2-5]. In recent scenario, tremendous effort has been done towards inorganic materials for the synthesis of nanoparticles towards a step into semiconductors due to its precise control and their size[6], shape[7], composition, crystal structures, strongly electronic charge carriers and also optical properties[8]. An attempt has been made to synthesize CdS and CdTe nanocrystals due to their semiconducting behavior and their unique properties[9,10]. The optical absorption for the CdTe nanocrystals is found to be at 1.5 eV. This concludes that the CdTe nanocrystals are ideal materials for photovoltaics, solar energy, X-ray, gamma ray detection and infrared detectors[11-13.]
Among all the transition metal oxides, CdTe is used for photovoltaic cells and semiconductors due to its low cost and having high absorption coefficient. Various experimental techniques have been introduced for the deposition of CdTe nanoparticles[14,15]. Rao et al. published their results on different materials in the earlier studies[16-65].
In the present study, an attempt has been made to prepare Ni^{2+} doped CdTe nanoparticles using co-precipitation method by varying the film properties through changing their composition. The obtained nanoparticles were characterized by spectroscopic techniques such as Optical, EPR and PL studies.

EXPERIMENTAL

Materials and Synthesis

Cadmium chloride ($CdCl_2$), Sodium hydrogen telluride (NaHTe), polyvinyl alcohol (PVA), Nickel Oxide (NiO) were purchased from Sigma Aldrich with 98% purity Ltd., India ,and double distilled water is used as a solvent. In present experimental method, 50 mL of double distilled water is taken in a 100 mL of beaker; 2.3g PVA and 0.045g of cadmium chloride were added in a beaker. Let the

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composite solution is left over without stirring for 24 hrs to swell at room temperature. Further, the obtained solution was allowed to heat on a hot plate up to 80°C with constant stirring up to 6 hours. After the continuous stirring highly viscous transparent solution was obtained. 1 mL of sodium hydrogen telluride (NaHTe) and 0.01 mol % nickel oxide was added drop wise into the solution, after few minutes a transparent solution is formed. The obtained viscous solution was coated on transparent glass slides and allowed to evaporate the solvent traces by placing in hot air oven. Finally, a thin film containing nickel doped PVA capped CdTe nanoparticles were obtained. The obtained nanoparticles were rinsed by ethanol to remove any impurities which are left on the surface of the nanoparticles before characterization.

Characterization

UV-visible spectrum was analyzed on to the prepared nanoparticles using JASCO V-670 Spectrophotometer. Electron paramagnetic resonance (EPR) spectrum was recorded on to the prepared nanoparticles by JEOL JES-FA series X-band EPR spectrometer. The current-voltage (I-V) and resistivity of the nanoparticles were studied using four-point probe measurement.Photoluminescence (PL) spectrum is taken for the prepared nanoparticles at room temperature on Horiba Jobin-Yvon Fluorolog-3 spectrofluorimeter.

RESULTS AND DISCUSSION

UV-visible Studies

TheOptical absorption spectra of Ni^{2+} doped PVA capped CdTe nanoparticles were analyzed by JASCO V-670 Spectrophotometer in the wavelength region 350-800 nm. Four bands of absorbance peaks are formed at 418, 722, 791 and 1198nm for nickel doped CdTe nanoparticles, which are clearly shown in Figure-1. Vibrational bands of Nickel ion, $Ni^{2+}(d^8)$ give rise to ^3F, ^3P, ^1D and several other singlet terms.^3F splits into $^3A_{2g}(F)$,$^3T_{2g}(F)$ and $^3T_{1g}(F)$ whereas ^3P transforms as $^3T_{1g}(P)$. The ^1D term splits into ^1Eg (D), $^1T_{2g}$ (D) and$^3A_{2g}(F)$ act as ground state of the crystal field[66]. The energy matrices of Nickel ion $Ni^{2+}(d^8)$ has been solved from the above assignments[67]. Inter electronic repulsion parametervalues were calculated using the following equations:

$$^3A_{2g}(F) \rightarrow {}^3T_{1g}(P) = 15Dq + 13.5B = \upsilon_1 \quad (1)$$
$$^3A_{2g}(F) \rightarrow {}^3T_{1g}(F) = 15Dq + 1.5B = \upsilon_2 \quad (2)$$
$$^3A_{2g}(F) \rightarrow {}^3T_{2g}(F) = 10Dq = \upsilon_3 \quad (3)$$

The evaluated values of Ni^{2+} doped PVA capped CdTe nanoparticles are observed at Dq = 835, B = 820 and C = 3150 cm^{-1}, which satisfies with the calculated values. Inter electronic repulsion parameters of observed and measured values are given in Table-1.The obtained value of inter-electronic repulsion parameter (B) is found to be the lowest form the observed values. This strongly suggests that the existence of a covalent bond formation between doped Ni^{2+} ions and its ligands.

Table-1: Optical band positions, crystal field and inter-electronic repulsion parameters of Ni^{2+} doped PVA capped CdTe nanoparticles

Transaction from $^3A_{2g}(F)$ ↓	Wavelength (nm)	Wavenumber (cm^{-1})		Dq (cm^{-1})	B (cm^{-1})	C (cm^{-1})
		Observed	Calculated			
$^3T_{1g}(P)$	418	23,942	23,923	835	820	3150
$^3T_{1g}(F)$	722	13,848	13,851			
$^1E_{1g}(D)$	791	12,654	12,642			
$^3T_{2g}(F)$	1198	8,336	8,347			

EPR Studies

Electron paramagnetic resonance is extreme sensitivity microscopic used for the characterization of metal particles and paramagnetic center of nanoparticles when diminished to nanoscale on JEOL JES-FA series having 100 kHz field modulation at room temperature. Figure-2 shows that EPR spectrum of Ni^{2+}

doped PVA capped CdTe, and an intense resonance signal is found at g = 2.23 (100 K) temperature and this value concludes that $Ni^{2+}(d^8)$ ions have octahedral coordination and orbital singlet $^3A_{2g}$ has the lowest energy level, which split into ^3F ground state as a consequence of crystal field.

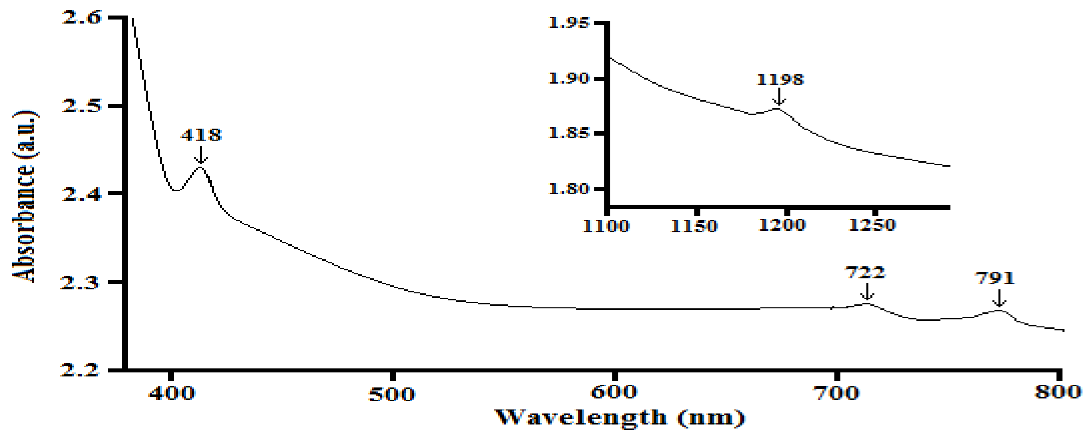

Fig.-1: Optical absorption spectrum of Ni^{2+} doped PVA capped CdTe nanoparticles

Using spin-Hamiltonian: H = gβHS with S = 1 and an isotropic g factor, an isotropic line is obtained which corresponds to the |0–1› |±1› magnetic dipole transitions[68]. Spin-orbit coupling of ligand field theory is given by the relation:

$$g = g_e - 8\lambda/\Delta \qquad (4)$$

Where λ is the effective spin–orbit coupling constant (207 cm^{-1}), g is an isotropic factor, g_e free electron value and Δ is the energy difference between the ground state $^3A_{2g}(F) \rightarrow {}^3T_{2g}(F)$.

Isotropic factor 'g' value is obtained from the above relation and it is found to be at 2.23. From optical studies, the Δ value is 8415 cm^{-1}. On comparison of an optical and isotropic factor the free ion value lies at 62% and wavelength λ = -335 cm^{-1}, this suggests a strong covalence bond formation. The Owens's ionic parameter α^2 can be evaluated by correlating the spectral peaks of EPR and optical data and the ionic parameter is calculated by the following equation:

$$g = 2.0023 - (\alpha^2 8\lambda/\Delta) \qquad (5)$$

The value of α^2 between 0.5 and 1.0 clearly indicates the limitation of pure ionic and covalent bonding. In the present study, the calculated value of α^2 is 0.62, which suggests that there exist a covalent bonding between doped Ni^{2+} ions and their ligands.

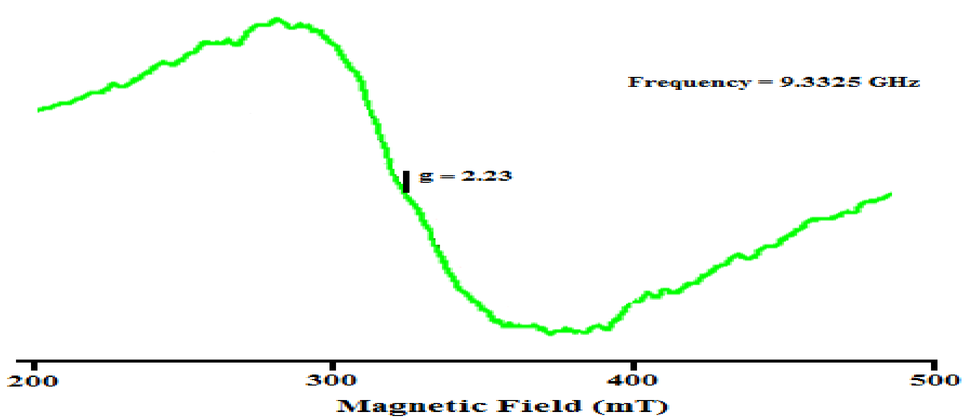

Fig.-2: EPR spectrum of Ni^{2+} doped PVA capped CdTe nanoparticles

I-V Characteristics

The current-voltage (I-V) and resistivity of the thin films and nanoparticles were studied using a four-point probe measurement with the Lucas Signatone system. I-V characteristics of Ni^{2+} doped PVA capped

CdTe nanoparticles are shown in Fig.-3 and Fig.-4. An increase in current with an increase in dopant concentration is observed due to the increased filling fraction. The electrical conductivity at room temperature could be varied by varying the CdTe content in PVA matrix, which makes them attractive for electronic technology[69].The charge-transference mechanism in PVA encapsulated CdTe system proposed by Greenham et al.[70]. The charge transport of ions takes place through the nanoparticles on to the prepared sample, when an electron hole pair gets rapidly separated with electrons which are attracted towards the nanoparticle, and pinholes on the polymer. It could be inferred that the PVA-CdTe composite behaves like a semiconductor. Fig.-3 demonstrates the current versus voltage behavior in the dark, while Figure-4 demonstrates the light condition. The dark current in the reverse bias is very close to zero which could be considered as an ideal case for diode characteristics.

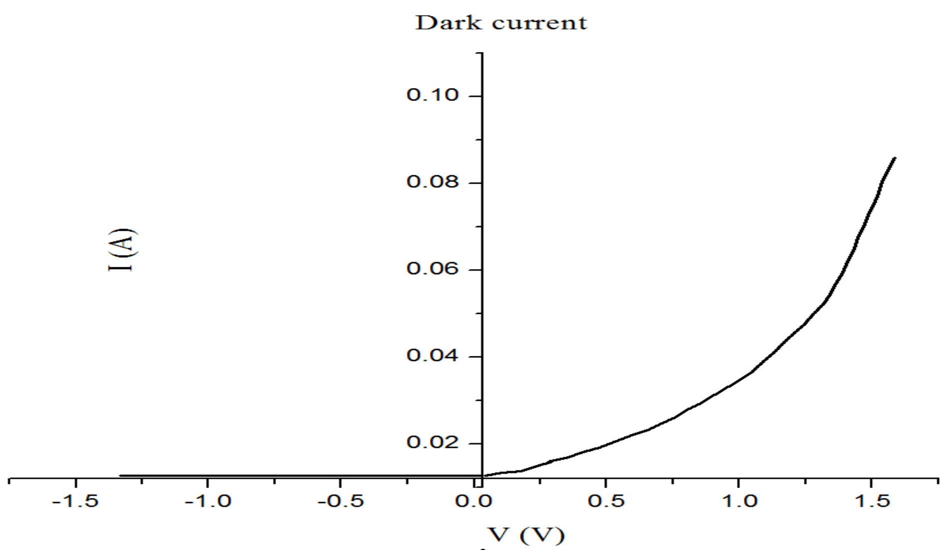

Fig.-3: I-V Curve of Dark Current for Ni^{2+} doped PVA capped CdTe nanoparticles

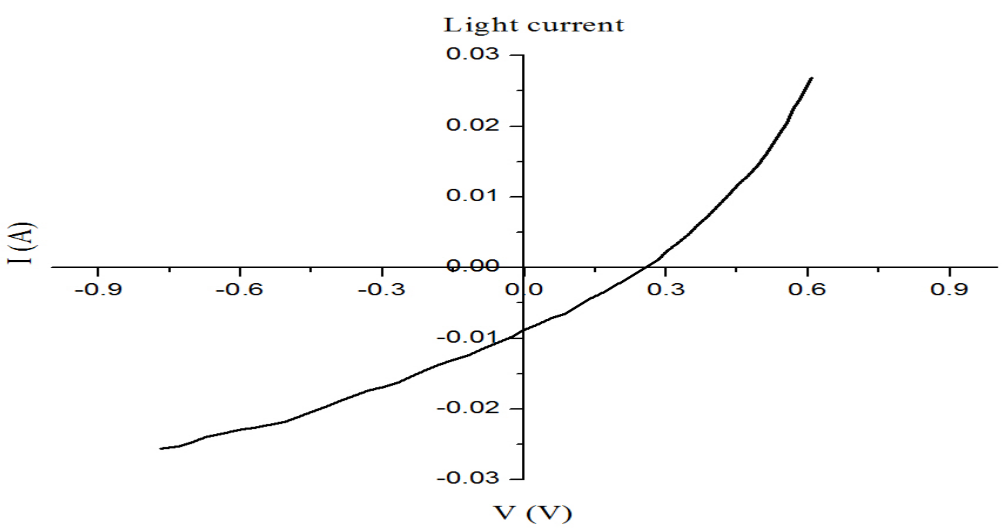

Fig.-4: I-V Curve of Light Current for Ni^{2+} doped PVA capped CdTe nanoparticles

Photoluminescence Studies

Photoluminescence spectrum is taken at room temperature on Horiba Jobin-Yvon Fluorolog-3 spectrofluorimeter with Xe continuous (450 W) and pulsed (35 W) lamps as excitation sources.PL spectrum reveals the information about the complexation of organic elements. Figure-5 shows luminescence properties of Ni^{2+} doped PVA capped CdTe nanoparticles and observed the two bands around 425, 467 nm at an excitation wavelength of 325 nm at room temperature. These bands are corresponding to violet and blue emissions in the visible region are important for the optoelectronic device applications.

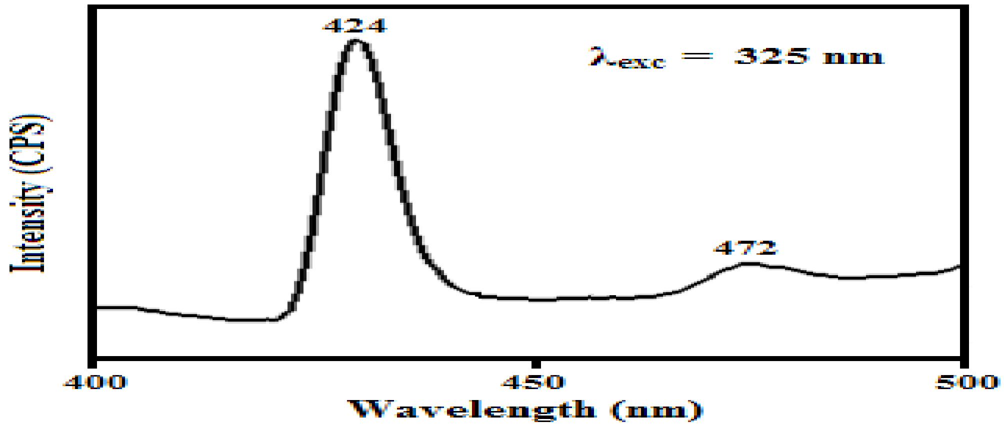

Fig. -5: PL spectrum of Ni^{2+} doped PVA capped CdTe nanoparticles

CONCLUSION

Ni^{2+} doped PVA capped CdTe nanoparticles were prepared by co-precipitation method. Optical absorption spectrum shows four characteristic bands of octahedral site symmetry; this agrees with the EPR studies. PL spectrum of Ni^{2+} doped PVA capped CdTe nanoparticles shows violet and blue emission. The PVA-CdTe composite behaves like a semiconductor. The dark current in the reverse bias is very close to zero which could be considered as an ideal case for diode characteristics. The obtained results of Ni^{2+} doped PVA capped CdTe nanoparticles are useful for making in LCDs, plasma devices, and electrochromic devices.

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