Structural Studies on PVA Capped CdS Nanoparticles

M.C. Rao¹, K. Ramachandra Rao²

¹Department of Physics, Andhra Loyola College, Vijayawada-520008, A.P., India
²Crystal Growth and Nano Science Research Centre, Department of Physics, Government College (A), Rajahmundry-533105

*Corresponding author: raomc72@gmail.com

Abstract: Nanometer-sized semiconductor particles belong to a state of matter in the transition region between molecules and solids. The colour tunability of semiconductor nanoparticles as a function of size is one of their most attractive characteristics. The control and improvement of the luminescence properties of quantum dots have been a major goal in synthetic procedures of nanoparticles. Cadmium sulphide is one of the most studied materials with a band gap of 2.43 eV. It is primarily used in solar cell and a variety of electronic devices. The photoconductive and electroluminescent properties of cadmium sulphide have been applied in manufacturing a variety of consumer goods. PVA has excellent film forming, emulsifying and adhesive properties. PVA capped CdS nanoparticles have been prepared at room temperature. The structural and optical absorption studies have been carried out on PVA assisted CdS nanoparticles. The average size of the particle is found to be less than 20 nm from the structural measurements. The absorption spectrum of the nanoparticles of CdS exhibited a well-defined absorption peak at 476 nm which is considerably blue-shifted relative to the peak absorption of bulk CdS indicating quantum size effect.

Keywords: CdS Nanocrystals, PVA, Structure.

1. Introduction

Nanometer-sized semiconductor particles belong to a state of matter in the transition region between molecules and solids. During the past two decades, research on quantum size semiconductor particles has increased enormously due to their exciting novel properties. The colour tunability of semiconductor nanoparticles as a function of size is one of their most attractive characteristics. The control and improvement of the luminescence properties of quantum dots have been a major goal in synthetic procedures of nanoparticles. Semiconductor nanoparticles have attracted much interest during the past decade due to their unique size dependent chemical and physical properties [1, 2]. Many synthetic methods, which normally include arrested precipitation in homogeneous solution and synthesis in confined reaction vessels such as reverse micelles and vesicles, have been developed for the chemical preparation of relatively mono-disperse nanoparticles of various semiconductor materials. Colloidal methods provide effective routes for preparing semiconductor nanocrystals that are soluble in organic solvents and which have a narrow size distribution. Surface chemistry is an efficient tool not only to organize and immobilize the nanocrystals, but also to effectively modify the emission properties. It is also possible to manipulate the synthesized nanocrystals by proper modification of the surface using capping agents thereby rendering them compatible in almost any chemical environment [3-5].

The synthesis of binary chalcogenides of group II-VI semiconductor in a nanopowder form has been a rapidly growing area of research due to their important optical, physical and chemical properties. These II-VI semiconductor nanoparticles are presently of great interest for their physical applications such as zero-dimensional quantum confined materials and for their applications in optoelectronics. Semiconductor nanoparticles belong to state of matter in the transition region between molecules and solids. Cadmium oxide is attracting tremendous attention due to its interesting properties like direct band gap of 2.3 eV. It is widely used in the applications like the preparation of cadmium-coated baths and manufacture of paint pigments. Cadmium sulphide is one of the most studied materials with a band gap of 2.43 eV. It is primarily used in solar cell and a variety of electronic devices. The photoconductive and electroluminescent properties of cadmium sulphide have been applied in manufacturing a variety of consumer goods. Polymers are chosen as good host materials because they usually exhibit long term stability and possess flexible reprocess ability. In addition, the small size and high optical activity of CdS nanoparticles make them interesting for optoelectronic applications operating in the ultraviolet region. In the case of semiconductor nanoparticles, radiative or nonradiative recombination of an exciton at the surface states becomes dominant in its optical properties with a decrease of particle size. These size dependent optical properties have many potential applications in the areas of solar energy conversion, light-emitting devices, chemical sensors, biological sensors and photo catalysis [6].

Polyvinyl alcohol (PVA) is produced commercially from polyvinyl acetate, usually by a continuous process. PVA has excellent film forming, emulsifying and adhesive properties. It is also resistant to oil, grease and solvent. It is nontoxic. It has high tensile strength and flexibility, as well as high oxygen and aroma barrier properties. However these properties are dependent on humidity, in other words, with
higher humidity more water is absorbed. The water, which acts as a plasticizer will then reduce its tensile strength but increase its elongation and tear strength.

2. Experimental

Cadmium chloride (CdCl₂) 99 mM of 4 mL is added to 2.2 g PVA (13,000 g/mol). The volume of solution is made up to 50 mL by bi-distilled water and the solution is left for 24 hours at room temperature to swell. After that the solution is warmed up to 80°C and stirred for 4 hours until viscous transparent solution is obtained. One millilitre of Sodium Sulphide (50 mM) is dropped into the solution with gentle stirring. Solution is casted on flat glass plate dishes. After the solvent evaporation, a thin film containing PVA capped CdS nanoparticles are obtained. The film is washed with de-ionized water to remove other soluble salts before measurements [7].

3. Results and Discussion

The XRD pattern of PVA capped CdS nanoparticles are recorded on PANalytical Xpert Pro X-ray powder diffractometer using CuKα (1.54060 Å) radiation. The XRD is used to determine the degree of crystallinity of PVA capped CdS nanoparticles using Debye-Scherrer’s equation [8] to estimate the particle size of the CdS nanoparticles. Depending on the full-width at half-maximum of diffraction peaks. As the particle size increases the broadening increases. The average size of the particle is measured by using Scherrer’s formula with the full width at half maximum intensity of the pattern.

\[ t = 0.9 \frac{\lambda}{\beta \cos \theta} \]

Where ‘t’ is the thickness, ‘\( \lambda \)’ is the wavelength of the radiation, ‘\( \beta \)’ is the full width at half maximum intensity (FWHM) and ‘\( \theta \)’ is the angle measured. The average size of the particle is found to be less than 20 nm. The lattice parameter (a) of the unit cells is calculated according to the relation:

\[ \frac{1}{d^2} = \frac{1}{a^2} (h^2 + k^2 + l^2) \]

Where, \( d \) is the interplaner spacing of the atomic planes as determined from the position of the peak (111), lattice parameter is estimated in the range of 5.34 – 5.40 Å. These values are smaller compared to the bulk value of 5.44 Å. As already mentioned the XRD peak broadening could also be due to the strain in addition to the crystalline size of the particle.

The most dramatic property of semiconductor nanoparticles is the size evolution of the optical absorption spectra. Hence UV visible absorption spectroscopy is an efficient technique to monitor the optical properties of quantum-sized particles. The absorption spectrum of the nanoparticles of CdS exhibited a well-defined absorption peak at 476 nm which is considerably blue-shifted relative to the peak absorption of bulk CdS indicating quantum size effect. The well-defined maximum at 476 nm is assigned to the optical transition of the first excitonic state. Generally, this wavelength of the maximum exciton absorption decreases as the particle size decreases as a result of quantum confinement of the photo generated electron hole pairs.

4. Conclusion

CdS nanoparticles could be used as good photo catalysts. Nanoparticles of CdS are synthesized through chemical precipitation technique at room temperature. The structural studies have been carried out on PVA capped CdS nanoparticles. The crystal structure and grain size of the particles are determined using XRD. The XRD studies revealed that the average size of the particle is found to be less than 20 nm. The lattice parameter is evaluated in the range of 5.384 – 5.40 Å. The absorption spectrum of the nanoparticles of CdS exhibited a well-defined absorption peak at 476 nm which is considerably blue-shifted relative to the peak absorption of bulk CdS indicating quantum size effect.

References