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Physical Properties of VO^{2+} and Cr^{3+} doped PVA Capped ZnSe Nanoparticles

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Abstract: ***Doped one-dimension semiconductor nanostructures are especially attractive for their unique optical and optoelectronic properties. As one of the most important group II-VI semiconductors, ZnSe with the bulk crystal transition energy of 2.7 eV at 300 K. VO^{2+} and Cr^{3+} doped ZnSe nanoparticles are synthesized by a simple chemical method using polyvinyl alcohol as a surface capping agent. The main advantage of this method is the use of nontoxic precursors and double distilled water as a solvent. For the prepared sample different physical parameters like refractive index, density, ionic concentration and electronic polarizability are measured and the correlation between these parameters is discussed.***

Keywords: VO^{2+}, Cr^{3+}, ZnSe, PVA and Physical parameters.

1. Introduction

Semiconducting nanomaterials exhibit many physical phenomena with some novel optical and transport properties, which are potentially useful for technological point of view especially in light emitting diodes, piezoelectric devices and photo detectors. Zinc selenide (ZnSe) belongs to the most promising wide band gap materials of the II-VI type and it is widely used in the fabrication of devices of semiconductor electronics and information display systems. It is necessary to note that a relatively high effective atomic number Zeff = 32 and a band gap width of Eg = 2.7 eV at 300 K make zinc selenide a promising material for the fabrication of X-ray detectors, which do not need cooling [1]. Nanocrystals synthesized by chemical route gives the chance to control their size, distribution and the most important is to improve the crystallinity.

Polyvinyl alcohol (PVA) is a bio-friendly polymer since it is water soluble and has extremely low cytotoxicity. This allows a wide range of potential biomedical applications. It is used as a stabilizer due to its optical clarity which enables investigation of nanoparticle formation. The refractive index of a material is an important optical parameter since it exhibits the optical properties of the material. Its values are often required to interpret various types of spectroscopic data.

The refractive index coefficients are important parameters in the design of a solid state laser. The instrument used to measure the refractive index is called refractrometer. Although many types of refractometers are available but the most common instrument is the Abbe's Refractometer. Density of solids is mostly the simplest physical property that can be measured. However, it would be a highly informative property if the structure of the material could be well defined. Density data is used to calculate the volumes of structural units. The densities of prepared samples are measured by using HT density measurement kit. Recently we have reported the physical properties of transition metal ions (Mn^{2+}, Fe^{3+} and Cu^{2+}) doped PVA capped ZnSe nanoparticles [2]. In the present study we discuss the physical properties of VO^{2+} and Cr^{3+} doped PVA capped ZnSe nanoparticles and the correlation between different parameters.

2. Experimental

0.054 g of Zinc chloride ($ZnCl_2$) was added to 2.2g PVA and volume of the solution was completed to 50 mL by double distilled water. The complete solution was left for 24 hours at room temperature to swell. The solution was warmed up to 60 ^{0}C and stirred for 4 hours until viscous transparent solution was obtained. One milliliter (mL) of Sodium Hydrogen Selenide (NaHSe) (50 mM) was dropped into the solution with gentle stirring and then 0.01 mol % transition metal ions were added to it to get transparent solution. The prepared solution was casted on flat glass plate dishes. After the solvent evaporation, transition metal ions doped PVA capped ZnSe nanoparticles were obtained [3]. The prepared film was washed with de-ionized water to remove other unsoluble salts before measurements.

3. Results and Discussion

The physical properties of transition metal ions VO^{2+} and Cr^{3+} doped ZnSe can be investigated by measuring their basic physical parameters like density and refractive index. The density and refractive index are the most important parameters for calculating the other parameters such as optical dielectric constant, molar refractivity, ionic concentration, electronic polarizability, inter-ionic distance and polaron radius etc. The physical transport properties of semi- conducting materials are very interesting and provide useful information regarding the structure and conduction mechanism.

The dielectric constant (ε) can be calculated by using the

refractive index given by

$\varepsilon = nd^2$

The reflection loss can be computed from refractive index using Fresnel`s formula

$R = [(nd-1)/(nd+1)]^2$

The molar refractivity RM can be evaluated using

$RM= [(nd^2-1) / (nd^2+2)] M/D$

where M is the average molecular weight and D is density in g/cc. The electronic polarizability αe can be expressed as

$\alpha_e = 3(nd^2 - 1) / 4\pi N (nd^2 + 2)$

where N is the number of transition metal ions per unit volume.

The inter-ionic separation and polaron radius can be determined as

$r_i = (1/N)\ 1/3$

$r_P = (1/2)\ [\pi / 6N]^{1/3}$

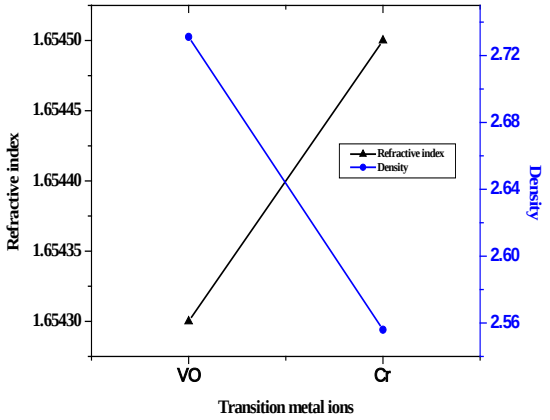

Figure 1: Correlation plot of density and refractive index of VO^{2+} and Cr^{3+} doped PVA capped ZnSe

By using the measured values of refractive index and density, other physical parameters are evaluated for VO^{2+}, Cr^{3+}doped PVA capped ZnSe nanoparticles by using different formulae and the correlation between different parameters are drawn.
By correlating these plots it is observed that the refractive index is high for Cr^{3+} whereas density is high for VO^{2+}. Generally refractive indices of polymer based materials vary in between 1.3-1.7. From Fig. 1 it is observed that both density and refractive index are out of phase with each other. From Fig. 2 it is observed that both electronic polarization and ion concentration also out of phase for both VO^{2+} and Cr^{3+}.

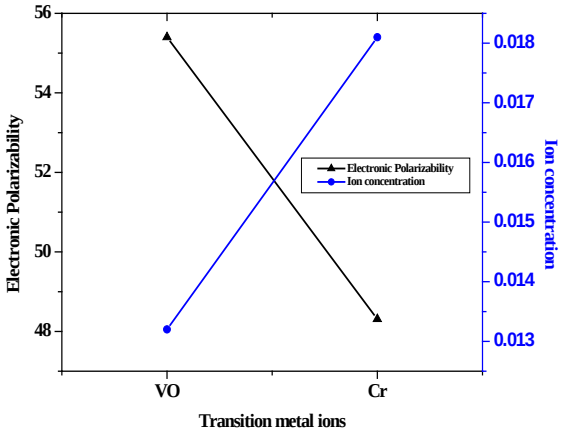

Figure 2: Correlation plot of ion concentration and electronic polarizability of VO^{2+} and Cr^{3+} doped PVA capped ZnSe

4. Conclusion

Correlations between different physical parameters reveal that density versus refractive index, electronic polarizability versus ion concentration is out of phase with each other. It is observed that if the sample is having low dielectric constant it is having high thermo-mechanical property. High refractive index polymer based materials are used in applications such as storage disc photonic crystal and high wave guides.

References

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