

Chapter: 6

Conclusion

ZnS, ZnS:Mn, ZnS:Ni nanoparticles were synthesized at different weight percentage of Mn and Ni with PVA as matrix. This method is simple and low-cost and hence it is suitable for industrial large scale production. The structural characterization of the nanomaterials were done with the help of XRD, TEM, SEM, SAED and the grain sizes are in well agreement in all the observations. EDX report confirms the doping of the elements. Optical characterization was done with UV-VIS spectrophotometer. The photoluminescence studies reveal the information of doped as well as un-doped nanoparticles. The sharp peak of Raman spectra indicated ZnS in well crystalline state which is in good agreement with that obtained from XRD result. The following conclusions can be made from the experimental observation.

6.1 Conclusion:

- 1) The structure of the nanoparticle so formed was found to be matching with JCPDS-Card No-50-0566, ($\lambda = 1.5405$, Zinc blende, $\text{CuK}\alpha$, system= cubic face centred). The structural characterization from XRD showed the cubic structures with diffraction peaks at (111), (220) and (311) for ZnS, ZnS:Mn and ZnS:Ni. Using Debye Scherrer's formula, the crystal size of ZnS, ZnS:Mn, ZnS:Ni nanoparticles were calculated and the average particle were found to be 2.88 nm, 2.45 nm, 2.92 nm respectively.

- 2) The formation of ZnS and ZnS:Mn nanocrystallites were confirmed by TEM (JEOL 2000 FX 11) micrograph. The particles were found to be spherical in shape and the average particle size for ZnS, ZnS:Mn, ZnS:Ni obtained from TEM were 5 nm, 2.5 nm, 4.04 nm respectively.

- 3) The surface morphology also studied with SEM where the particles were found to be spherical in shape in case of ZnS:Mn and ZnS:Ni. The cubic structure of ZnS is observed.

- 4) The elemental percentage analyses of the ZnS:Mn and ZnS:Ni carried out by EDX agreed well with the theoretical consideration.

- 5) Using Brus equation the particle sizes for ZnS, ZnS:Mn, ZnS:Ni obtained are almost identical with that obtained using Debye Scherrer's formula.

- 6) Photoluminescence studies confirmed the presence of dopant in the nano crystallites. The PL study indicates that both Mn and Ni act as electron trapping centres and this results nonradiative recombination and hence the luminescence intensities decreases because of S^{-2} .

- 7) The broadened and increase of PL intensity at 0.25% doping for suggests more incorporation in ZnS. The broadened emission band with multiple of peaks maxima is because of the involvement of different luminescence centres in the irradiative process.
- 8) The yellow emission is due to incorporation of Mn into the ZnS lattice and was found at 581 nm which was also a confirmation successful Mn doping. Starting with the blue emission (at 478 nm), intensity decreases towards the orange emission (at 581nm) for 0.5%, 0.75% 1.0% doping while there is an increase in intensity at 581 nm for 0.25% doping.
- 9) From the stable crystal structure and crystal size, it can be assumed that Zn and Ni ions are similar in size (mentioned in table). This also indicates the absence of impurity phases at the concentrations 0%, 0.25%, 0.50%, 0.75% and 1.0%.
- 10) The broadening of PL peaks for ZnS:Mn is more than ZnS:Ni, which indicates that more incorporation of ZnS in ZnS:Mn than ZnS:Ni.
- 11) Double Beam Automated Spectrophotometer (Hitachi – U3210) [UV-Visible spectrometer] was used to calculate the band gap. For both ZnS:Mn and ZnS:Ni the band gap were found be higher than bulk ZnS. The peaks for ZnS:Mn and ZnS:Ni showed a tendency towards blue shift. It is also observed that with the doping concentration from 1.00% to 0.25%, the band gap increases.

- 12) The increase of band gap energies from 3.68 eV to 3.90 eV with increase in doping percentage indicate the blue shift of ZnS:Mn which is also an indication of quantum confinement effect due to decreasing size of nanostructure.
- 13) For ZnS:Ni the increase of band gap energies from 3.52 eV to 3.86 eV with increase of doping percentage indicate the blue shift of ZnS:Ni which is occurs because of quantum confinement effect as size decreases.
- 14) Raman spectra indicated ZnS in well crystalline state. The peaks at 58 cm^{-1} and 335 cm^{-1} , 347 cm^{-1} are the characteristic Raman scattering of ZnS and indexed to LO phonon mode. Another peak at 264 cm^{-1} corresponds to TO phonon mode of ZnS.
- 15) There is an increase of particle sizes for both Mn and Ni doping (at 1% doping is observed compared to 0.25% doping) which may be due to the agglomeration.
- 16) For the 0.25% doping percentage is more effective in respect of particle size which is one fundamental requirement in nanoparticles. Blue and green emission at 0.5% to 1.0% indicate large band gap which has industrial application. The low band gap at 0.25% emits red colour which may be also a good industrial application.
- 17) This method is simple and low-cost and hence it is suitable for industrial large scale production.

18) In between ZnS:Mn and ZnS:Ni, it is found that the particle size of ZnS:Mn, is smallest i.e. 2.45 nm from the reports of XRD, and 2.5 nm from TEM report and are equal in size.

19) For the 0.25% doping percentage is more effective in case of reducing particle size which is one fundamental requirement in nanoparticles. Blue and green emission at 0.5% to 1.0% indicate large band gap which has industrial application. The low band gap at 0.25% emits red colour which may be also a good industrial application.

20) Zinc sulfide is also used as an infrared optical material, transmitting from visible wavelength to just over 12 micrometers. It can be used planar as an optical window or shaped into a lens. It is made as microcrystalline sheets by the synthesis from hydrogen sulfide gas and zinc vapors. and FLIR-grade (Forward Looking IR), where the zinc sulfide is in a milky-yellow, opaque form.