EFFECT OF MN CONTENT ON THE STRUCTURAL AND OPTICAL PROPERTIES OF CO-PRECIPITATED MN –ZNO NANOPARTICLES

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I. Abstract:

Metal oxide nanoparticle applications in energy storage device which receive attention for the future energy requirement. These transition metal oxides, when falling in the nanosized that process more applications in the field such as data storage, spintronics, biomedicine and telecommunication. Mn-ZnO nanoparticles were synthesized by Co Precipitation method. The oxalic acid solution drop wise added to the metal salt solution with continuous stirring to get light pink precipitate dried at 100^0C . The synthesized powder was calcined at various temperatures. Such as 200^0C, 300^0C, 400^0C to obtain block color Mn-ZnO nanoparticles. These particles thus prepared were characterized by FTIR, UV-Visible. The optical band gap of Mn-ZnO nanoparticle was estimated by UV-Visible Spectroscopy .The direct band gap values were found to be 2.1eV, 2.5eV, and 3eV.

Key words: Mn-ZnO, FTIR, UV, band gap.

II. INTRODUCTION

Despite the fact that a unique definition does not exist for nanoparticles, are They usually referred to as particles properties of the material don't just scale down physical or up, with a size up to 100 nm. It can be argued that below that size, the physical properties of the material don't just scale down or up, but change. Nanoparticles exhibit completely new or improved properties based on specific characteristics (size, distribution, morphology, phase, etc). If compared with larger particles of the bulk material they are made of nanoparticles can be made of a wide range of materials, the most common being metal oxide ceramics, metals, silicates and non-oxide ceramics. Even though nanoparticles of other materials exist, e.g. those based on polymer materials or compound semiconductors, the former categories count for the most part of current applications.

Nanoparticles present several different morphologies (flakes, spheres, dendritic shapes, etc.,) While metal and metal oxide nanoparticles in use are typically spherical, silicate nanoparticles have flaky shapes with two of their dimensions in the range of 100- 1000 nm. They are generally designed and manufactured with physical properties tailored to meet the needs of the specific application they are going to be used for.

III. EXPERIMENTAL TECHNIQUES

Cadmium doped ZnS nanoparticles were synthesized by co-precipitation technique. The above nanoparticles were characterized by using X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), optical absorption spectroscopy,

optical transmission spectroscopy and Fourier Transform Infra-Red Techniques (FTIR).

Co-precipitation reaction involves the simultaneous occurrence of nucleation, growth, coarsening and agglomeration process. There are three main mechanism of co-precipitation; inclusion, occlusion, and adsorption. An inclusion occurs when the impurity occupies a lattice site in the crystal structure of the carrier, resulting in a crystallographic defect; this can happen when the ionic radius and charge of the impurity are similar to those of the carrier. An adsorb ate is an impurity that is weakly bound (adsorbed) to the surface of the precipitate. An occlusion occurs when an adsorbed impurity gets physically trapped inside the crystal as it grows.

X-RAY DIFFRACTION (XRD) TECHNIQUE

X-ray powder diffraction (XRD) is rapid analytical technique primarily used for phase identify action of a crystalline material and can provide information on unit cell dimensions. The analyzed material is finely ground, homogenized, and average bulk composition is determined.

FOURIER TRANSFORM INFRARED (FTIR) SPECTROSCOPY.

Fourier Transform Infrared Spectroscopy (FTIR) is a powerful tool for identifying types of chemical bonds in a molecule by producing an infrared absorption spectrum that is like a molecular “fingerprint”. Because each different material is unique combination of atoms, no two compounds produce the exact same infrared spectrum. Therefore, infrared spectroscopy can result in a positive identification (qualitative analysis) of every different kind of materials. In addition, the size of the peaks in the spectrum is a direct indication of the amount of material present. With modern software algorithms, infrared is an excellent tool for quantitative analysis.

- It can identify unknown materials
- It can determine the quality or consistency of a sample

ULTRAVIOLET AND VISIBLE SPECTROSCOPY

We see sunlight (or white light) as uniform or homogeneous in color, it is actually composed of a broad range of radiation wavelengths in the ultraviolet (UV), visible and infrared (IR) portions of the spectrum.

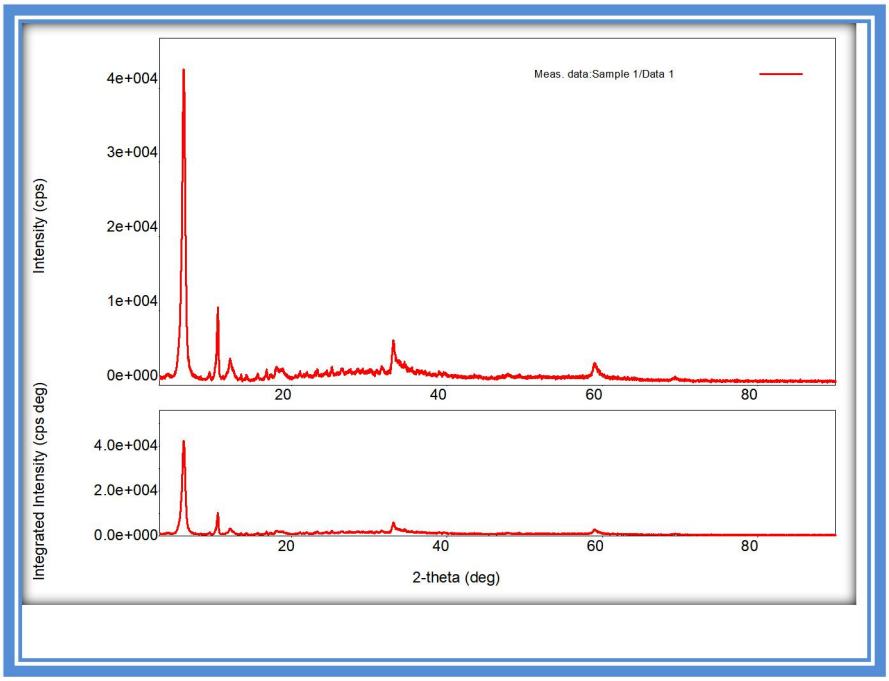
As shown on the right, the component colors of the visible portion can be separated by passing sunlight through a prism, which acts to bend the light in differing degrees according to wavelength as shown in Fig.2.8.Electromagnetic radiation such as visible light is commonly treated as a wave phenomenon, characterized by wavelength or frequency. Wavelength is defined on the left below, as the distance between adjacent peaks (or troughs), and may be designated in meters, centimeters or nanometers (10^{-9} meters). Visible wavelengths cover a range from approximately 400 to 800nm.

VI. RESULT AND DISCUSSION

X-Ray Diffraction method

$Zn_{1-x}Ni_xO$ nanocomposites. All the diffraction peaks of ZnO nanoparticles can be indexed to the hexagonally structured ZnO, and the interplanar spacing (d_{101}) is about 2.472 A^{o}, all in good agreement with standard card (JCPDS Card No.89-1397). The broading of the diffraction peaks indicated the formation of ZnO nanocrystallites. In addition, the strong peaks show the crystalline nature of the samples. Peaks positions of the MnO sample indicate the formation of the cubic structure with three most preferred orientation (1 1 1),(220), and (311), and the

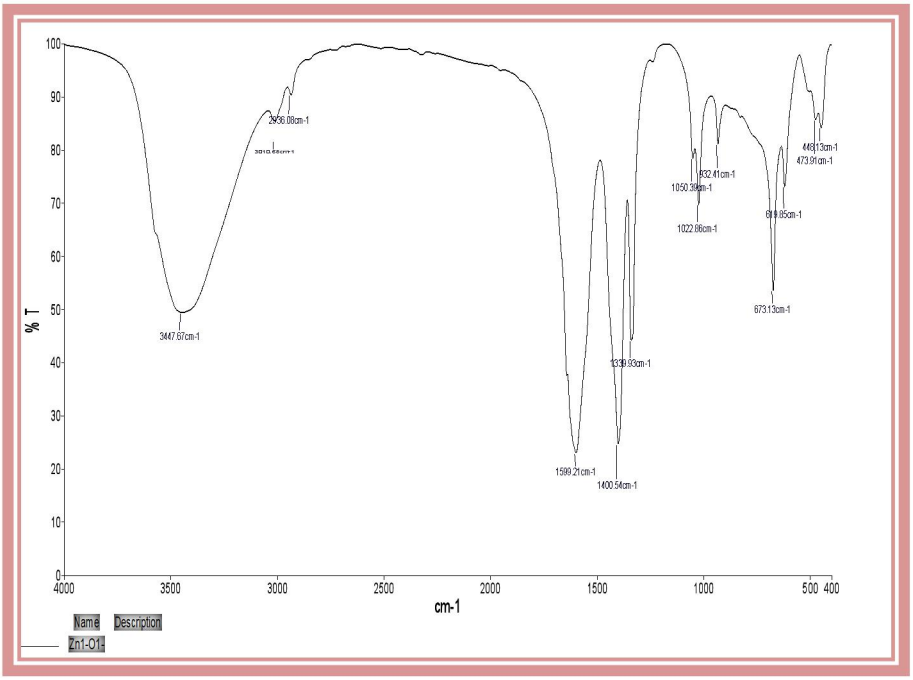
broadening of the diffraction peaks shows the formation of nanosized particles. The interplanar spacing of the d_{111} is about 3.379 A°, well in agreement with the standard card (JCPDS Card No. 89-0440). No diffraction peaks from the other crystalline forms were detected. The average size of nanocrystalilites is calculated from full width at half maximum of XRD peaks using Debye – Scherrer's formula (Caruso 2001). From the calculation, the average diameters of the particles are 0.26,0.22,0.35, undoped ZnO nanostructures, respectively. As seen in fig.1 a mixed structure was formed in different thickness of coated on ZnO composites. This shows the hexagonal (ZnO) as well as cubic (MnO) structures, implying that there is no change in crystal structure by the process. However, the relative intensity and FWHM are changed. This is the first time that the mixed structure of ZnO (Hexagonal) nanocomposites was obtained.



X-ray diffraction pattern of ZnO nanoparticles from 0° to 100°

Fourier transforms infrared (FTIR) studies

The characteristic peaks exhibited by FTIR spectra of $Zn_{1-x}Mn_xO$ (0, 0.2, and 0.3) nanoparticles from 380 to 3880 cm^{-1} at room temperature are shown in Fig 4, Fig 5, and Fig 6. It is obtain the information about the chemical bonding present in the material, identity and characterize the organic species and elemental constituting in the material. The characteristic peaks exhibited by, the IR frequencies along with the vibrational assignments of the nanoparticles assigned at room temperature are listed in Table 2.The broad absorption band around 3418 to 3447 $cm^{-1}$is assigned to the presence of normal polymeric O-H stretching vibration because all FTIR spectra are recorded by mixing samples with KBr. Hence there may be some absorbed water apour, as KBr is hygroscopic .



FTIR spectra of ZnO nanoparticleat room temperature in the wave number from 400 to 4000 cm^{-1}

ULTRAVIOLET AND VISIBLE SPECTROSCOPY

The optical absorption spectra have been observed by using UV-Visible-NIR(Varian Cary) spectrophotometer and the results are in fig .7. The characteristics absorption peaks due to undoped and Mn^{2+} doped ZnO Nanoparticles appear in the wavelength range 250-340nm.These peak positions reflect the band gap of nano particles and the synthesis ZnO Nanoparticles have no absorption in the visible region (800-400 nm).The fundamentals absorption, which corresponds to electron excitation from the valance band to conduction band, can be used to determine the value of the optical band gap of the synthesized ZnO nanoparticles. The relation between the incident photon energy (hν) and the absorption coefficient (α) is given by the following relation $\alpha h\upsilon = A(h\upsilon - E_g)^n$

Where A is constant and E_g is the band gap energy of the material

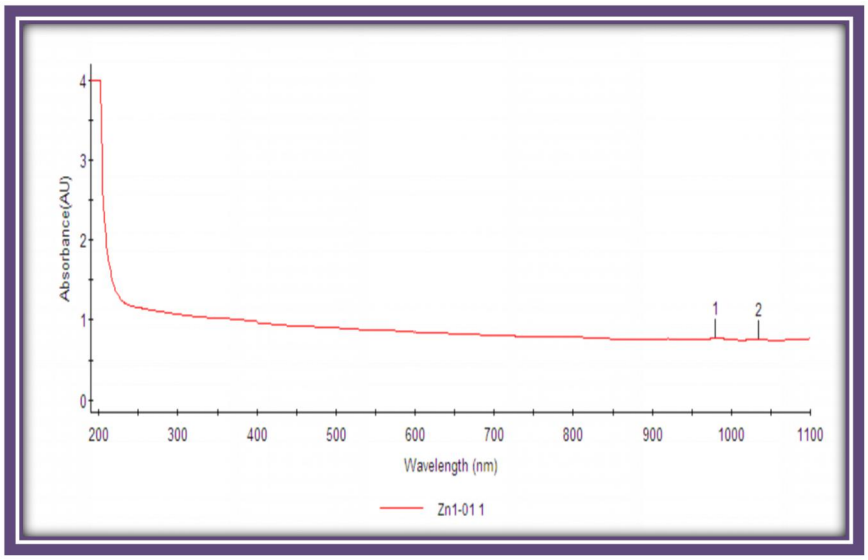


Figure 7. UV-Visible absorption spectra of ZnO nanoparticles.

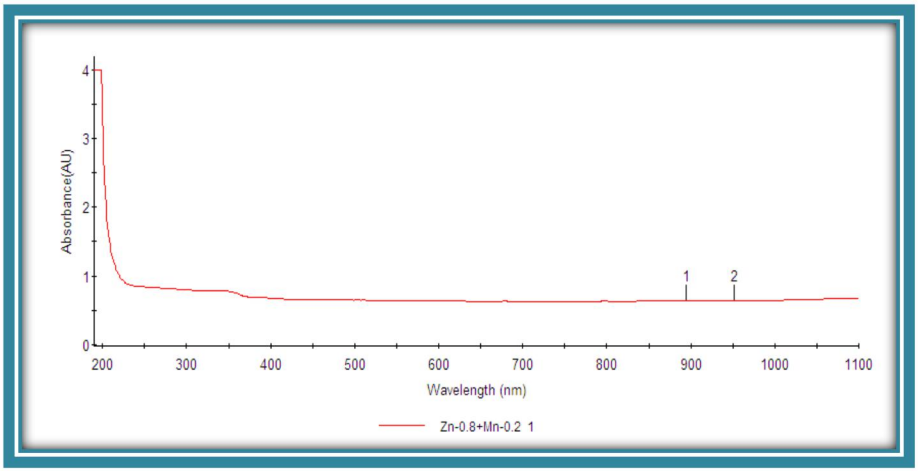


Figure 8. UV-Visible absorption spectra of $Zn_{0.8}$ $Mn_{0.2}$S nanoparticles.

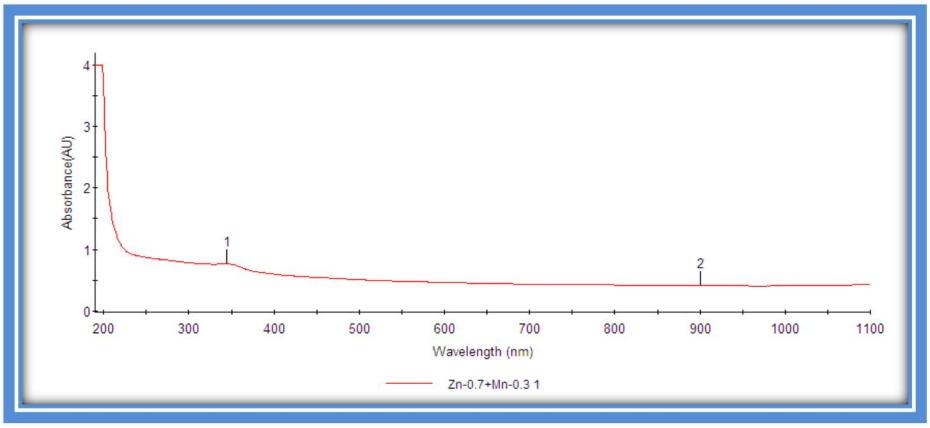


Figure 9. UV-Visible absorption spectra of $Zn_{0.7}$ $Mn_{0.3}$S nanoparticles.

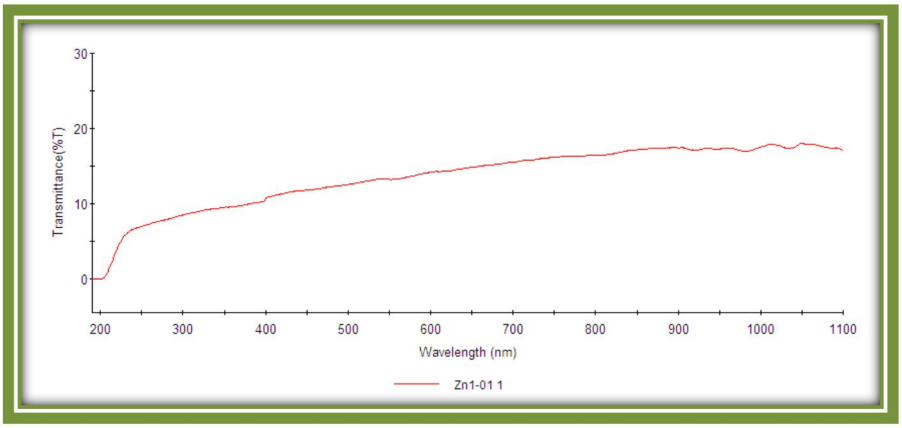


Figure 10. . UV-VisibleTransmittance spectra of ZnOnanoparticles

V. Conclusion

$Zn_{1-x}Mn_xO$ ($0.0 \leq 0.2 \leq 0.3$) nanoparticles were successfully prepared by chemical co precipitation method.

- ✓ Cubic zinc blende structure of the prepared nanoparticles was confirmed by XRD analysis. Due to the increase of Mn content into the nanoparticles, all the peaks shifted towards the higher diffraction angles.
- ✓ The substitution of Mn^{2+} ions into the Zn-O lattice is confirmed by the change in lattice parameters. The lattice constant also gradually decreased as Mn content increased.
- ✓ The particle size was calculated from the XRD result. It was maximum (0.16nm) for $Zn_{0.8}Mn_{0.2}O$, minimum (0.10 nm) for $Zn_{0.7}Mn_{0.3}O$.
- ✓ The observed shift in blue band of UV spectra confirmed the substitution of Mn into Zn-O lattice.
- ✓ The present result provides good indication of tuning the visible emission of the ZnO nanoparticles by the formation of ZnO core-cell nanoparticles.
- ✓ The weak peaks due to ZnO stretching are observed at about 450 cm^{-1} for $Zn_{0.7}Mn_{0.3}O$ andZnO bond is shifted to higher frequency as 473 cm^{-1}, and 472 cm^{-1} for $Zn_{0.8}Mn_{0.2}O$.

VI. BIBLOGRAPHY

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