

Study of blue shift in Iron (Fe) doped ZnO Nanoparticles at different Molarities by Wet Chemical Method

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Abstract – Iron (Fe) doped Zinc Oxide (ZnO) nanoparticle is a very important topic of study in the field of nanoscience and nanotechnology. We have prepared Iron doped ZnO nanoparticles by Wet chemical method. We report the optical properties of Iron (Fe) doped ZnO nanoparticles at different molarities (0.025M, 0.05M and 0.1M). The band gaps of all nanoparticles prepared at different molarities are calculated with the intercept on Y-axis of Tauc plot from UV absorption spectra using UV-Vis Absorption spectroscopy. It has been observed that band gap decreases as the molarity increases. At 0.025M, 0.05M and 0.1M band gap are found to be 4.9eV, 4.89eV and 2.7eV respectively. This reduction in band gap suggest that the band gap of prepared nanoparticles are shifted towards lower energy. This shifting in band gap the blue region gives the idea of blue shift quite well. This blue shift is dependent on the particle size of the nanoparticles.

Keywords -Blue shift, Band Gap, Optical properties, Wet Chemical technique, Molarity

I. INTRODUCTION

The nanoscale system and the special properties of the material in this range have attracted people throughout the world [1]. ZnO has a wide band gap of 3.3eV at room temperature. It is very useful material for different technological application like optical, optoelectronic devices, liquid crystal display [2, 3]. Due to Quantum size confinement, these nano materials due to their peculiar characteristics often show novel physical properties compared to those of the bulk one. Controlling the size and shape of the new one, it will be possible to enhance the properties. Out of all the methods for the fabrication of nanoparticle, we have applied wet chemical method [4], [5], [6] and [7], which is the most cost effective for large scale production. Here we report the syntheses of Iron (Fe) doped ZnO nanoparticles with and the blue shift of the optical band gap.

II. EXPERIMENTAL DETAILS

2.1 Materials and Methods

All materials are purchased from the commercial market with highest purity (99.99%). Zinc Acetate Dihydrate ($\text{CH}_3\text{COO}_2\text{Zn}2\text{H}_2\text{O}$) and Sodium Hydroxide (NaOH) as the starting materials, Polyvinyl Alcohol (PVA) as capping agent and double distilled water as dispersing solvent are used to prepare the ZnO thin film.

2.2 Preparation of ZnO nanoparticle in thin films:

In the experimental process the 0.1M, 0.05M and 0.025M solution of Zinc Acetate Dihydrate ($\text{CH}_3\text{COO}_2\text{Zn}2\text{H}_2\text{O}$) are stirred constantly for 1hour at 343K (solution 1,2,3). PVA is stirred constantly at 343K (solution 4, 5, 6) to prepare 0.1M, 0.05M and 0.025M solution. Now NaOH is slowly added drop by drop into the (solution 1, 2, 3) and stirred at room temperature for half an hour and white solutions is obtained as (solution 7, 8, 9). Again to prepare Iron (Fe) doped ZnO we prepare FeCl_3 solution separately of three different concentration 0.025M, 0.05M and 0.1M as (solution 10, 11, 12) and mixed with the solution of (4, 5, 6) and (7, 8, 9) to have solution (13, 14, 15). The thin films are deposited on glass substrate. Therefore Glass substrates are washed perfectly with some acid and then with distilled water and allowed to dry at room temperature. The substrates are dipped into the final solution (13, 14, 15) for 24 hour. After 24 hours the glass substrates are removed from solutions (13, 14, 15) and allowed to dry at room temperature.

III. CHARACTERISATION METHOD

The optical absorption spectra of ZnO are recorded by a UV-Vis spectrometer (HITACHI model U-3210). UV-Visible spectroscopy is the absorption spectroscopy in the ultraviolet-visible spectral region. It uses light nearby visible region.

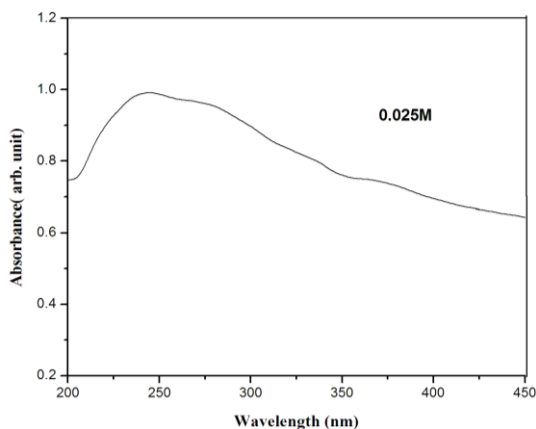


Figure 1

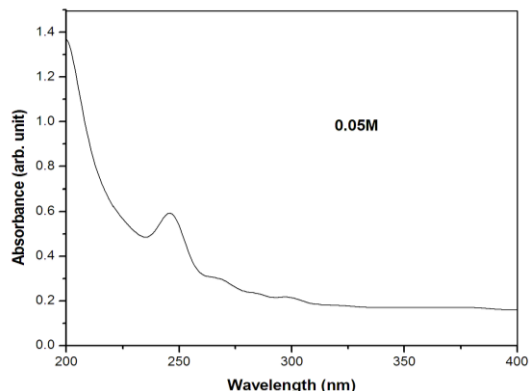


Figure 2

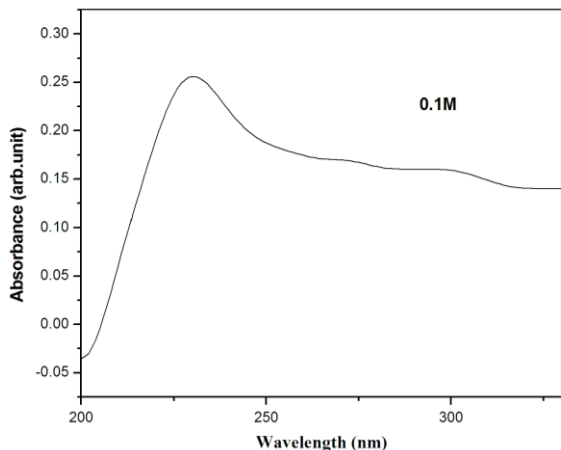


Figure 3

UV- VIS absorption spectra is used to find out changes in the energy band gap of ZnO due to iron doping. All the samples prepared at RT show absorption peak around 240nm. The absorption peak of the corresponding annealed shifts towards

the lower wavelength side or the peak is blue shifted. This blue shift is due to quantum confinement effect [8]. According to quantum confinement theory [9], the electrons in the conduction band and holes in the valence band are confined spatially by the potential barrier of the surface. Because of the confinement of electrons and holes, the optical transition energy from the valence top to the conduction bottom increases and the absorption maximum shifts to the shorter wavelength region. The stronger exciton effect is an important character of quantum confinement in nano semiconductors, in which the electrons, holes and excitons have limited space to move and their motion is possible for definite values of energies. Thus their energy spectrum is quantized [10]. The continuum of states in conduction and valence bands are broken into discrete states with an energy spacing relative to band edges which is approximately inversely proportional to the square of the particle size and reduced mass [11]. The highest occupied valence band and the lowest unoccupied conduction band are shifted to more negative and positive values respectively which results the increase in band gap, than the bulk value. Thus there will be a blue shift in the absorption spectra with reduction in crystallite size. Annealed ZnO nanoparticles show stronger UV-Vis absorbance than the as-grown ZnO nanoparticles.

The band gap energy of Iron doped ZnO is estimated from the graph of $h\nu$ versus $(\alpha h\nu)^2$ through the absorption coefficient α which is related to the band gap E_g as $(\alpha h\nu)^2 = k(h\nu - E_g)$, where $h\nu$ is the incident light energy and k is constant. The extrapolation of the straight line in Fig.f to $(\alpha h\nu)^2=0$ gives the value of the band gap E_g . The optical band gap are found to be size dependent and the band gap decreases as the particle size increases. The band gap energy of the samples is calculated by using the following equation

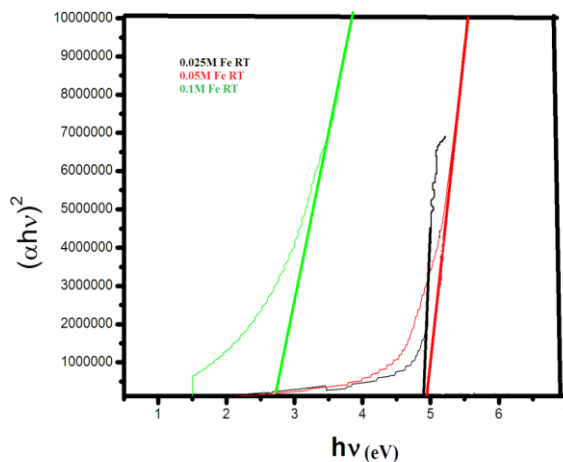


Figure 4

Figure 4 gives the tauc plot of Iron doped ZnO at RT. The band gap obtained for different doping concentration at RT.

Temperature/Concentration	0.025M	0.05M	0.1M
RT	4.90eV	4.89 eV	2.7eV

Table 1 Variation of band gap with molarity

The increase in band gap at 0.025M is due to the substitution of Zn²⁺ ions by Fe³⁺ ions which create additional free carriers moving the Fermi level towards the conduction band [10]. As the concentration is increased the band gap gradually decreases which is due to the addition of Fe as ZnO can change the Fermi Energy state by lifting valence band maximum as lowering the conduction band minimum leading to band gap reduction [11].

VI. CONCLUSION

ZnO nanoparticles have been prepared using wet chemical syntheses method and were characterized by UV-Vis absorption spectroscopy. The significant sharp absorption of UV radiation by ZnO nanoparticles indicates the monodispersed nature of the nanoparticle distribution. From UV-Vis absorption spectrum, the calculated average size of the prepared nanoparticles is found to be 0.8 nm corresponding to peak absorption wavelength 209nm. The band gap decreases with the ncrease in molarity. At 0.025M, 0.05M and 0.1M band gap are 4.9eV, 4.89eV and 2.7eV. Therefore it is confirm that as the molarity of the dopant increases band gap decreases. Thus we can cloude that increase in doping concentration decreases the space between conduction and the valence band. These ZnO nanoparticles can be used in different applications like sensors, active medium for lasers etc. In future we will try to implement these in some devices.

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