Study of different capping agents effect on the optical and morphological properties of ZnO nanoparticles

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Abstract: A co-precipitation method has been proposed to study of different capping agents effect on optical and morphological properties of zinc oxide nanoparticles. This method has clear advantages including simplicity and stability. The SPR peaks correspond to PEG and CTAB capped ZnO nanoparticles were compared when different capping agents are used. The obtained samples have been characterized by X-ray diffraction, UV-Visible absorption spectroscopy and Field Emission Scanning Electron Microscopy. The functional groups were studied for both PEG and CTAB capped ZnO nanoparticles by FTIR. The present work shows that capping agent is an important factor for controlling optical and morphology of the nanoparticles.

Keywords
PEG (Poly Ethylene Glycol)
CTAB (Cityl Trimethyl Ammonium Bromide)
Capping agents
Morphology

1. Introduction

Among the different nanomaterial, metal oxide nanomaterial has created an interesting technological and industrial effect. Especially zinc oxide nanoparticles have received a great attention because of its excellent advantages in electrical, magnetic and catalytic properties. ZnO nanoparticles has wide range of applications including solar cells[1], optoelectronics[2], field emission devices[3], gas censor[4] sun screen lotion, cosmetics[5] and spintronic devices[6]. ZnO nanoparticles are prepared by several methods such as solid state, hydrothermal, solvothermal and solution combustion synthesis[7-9]. Among these methods co-precipitation method gives as easy, time consuming and mass collection of nanoparticles. The surfactant plays an important role in material synthesis such as reduce the particles size, avoid the agglomeration of nanoparticles due to electrostatic interactions between particles. Once the capping agent is absorbed on metal oxide nanoparticles, the particle activity is controlled, which leads to reduce the particles aggregation. Moreover both CTAB and PEG are non-toxic, non- irradiative in nature.

In this present work the effect of encapsulating ZnO nanoparticles with different capping agents such as PEG and CTAB on optical, structural, morphological studies were compared. CTAB as a surfactant has been widely used in nanoparticle synthesis to control the particles size by capping the nanoparticles[10]. Also non-ionic PEG shows an efficient results on dispersability of the ZnO nanoparticles[11-12]. The main goal of this paper is to analyze the efficiencies of surfactant on optical, structural and morphology of zinc oxide nanoparticles.

2. Experimental details

2.1. Materials

All the chemicals used in this work were analytical grade reagents and used without further purification. Zinc chloride (ZnCl2), PEG (Poly Ethylene Glycol), CTAB (Cityl Trimethyl Ammonium Bromide) and sodium hydroxide (NaOH) were purchased from Merck company. Deionized water was used to prepare all solutions.

2.2. Preparations of PEG and CTAB capped ZnO nanoparticles

Zinc oxide nanoparticles were prepared by co-precipation method. Zinc chloride was taken as precursor, PEG and CTAB were taken as capping agents and NaOH was taken as precipitating agent. The required amount of zinc chloride (ZnCl2) was dissolved in 50 ml of de-ionized water and this solution was stirred for 1 hour in the magnetic stirrer. 5 gm of PEG (Poly Ethylene Glycol) was dissolved in 50 ml of de-ionized water and the solution was stirred for one hour. Then PEG solution was added to the precursor solution and the mixture was stirred for one hour at room temperature, and NaOH solution was added drop by drop to the mixture till reaches pH value 8. Then sample was stirred in the magnetic stirrer continuously for 8 hours and the precipitated solution was washed twice with de-ionized water and then with acetone. The solution was kept in constant temperature bath. The dried powder was grinded and calcinated under 400˚C for 5 hours. Finally the resulting PEG capped ZnO nanopowder was collected in a clean sample wile. The same procedure was followed to prepare CTAB capped zinc oxide nanoparticle

2.3. Characterization

The powder XRD analysis was carried out by Enraf Nonius CAD4-F diffractometer with the CuKa (λ=1.540AÅ) radiation. The Fourier infrared spectra (FTIR) were recorded in the range of 400- 4000 cm-1 on a Perkin-Elmer Spectrum II FT-IR spectrometer. UV-Visible absorption spectra were recorded at room temperature using a Varian Carey UV-Visible spectrophotometer from 200 nm to 1200 nm.

3. Results and discussion

3.1. UV-Visible spectral analysis

Figure 1. (a) and (b) show the optical absorption spectra of zinc oxide nanoparticles with different capping agents PEG and CTAB.The absorption peak is due to the SPR (Surface Plasmaon Resonance) absorption of zinc oxide nanoparticles,which is also used to analyze morphological property of the nanoparticles. The sharp SPR peaks clear that the particles are distrubuted uniformly. The absorbed

peaks of PEG capped ZnO and CTAB capped ZnO are lies below 400 nm and the SPR peaks are blue shifted and centred at 364 nm for PEG capped ZnO and 340 nm for CTAB capped ZnO.

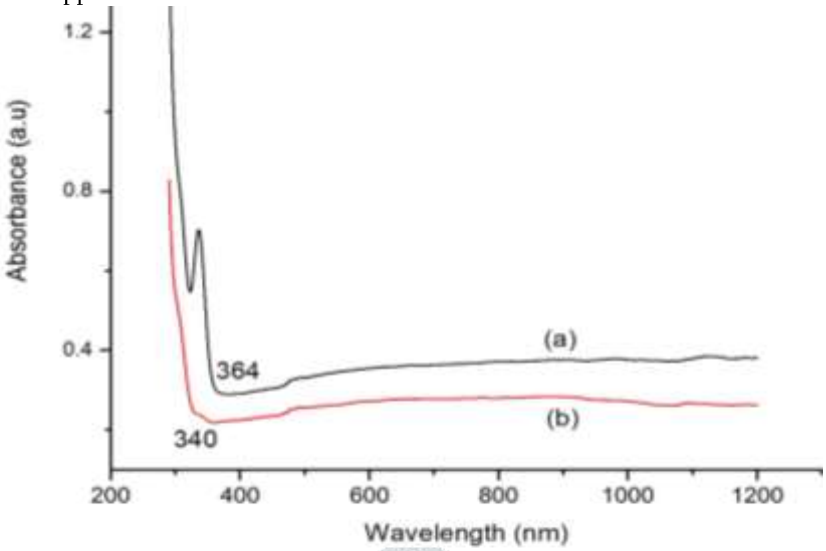

Fig 1.UV –Vis spectra of Zno nanoparticles calcinated at 400 °C (a) PEG (b) CTAB capped ZnO

The band gap energy of ZnO nanoparticles are calculated from energy wave equation,

$$E=hc/\lambda.$$

Where h is the planck's constant, c is the velocity of light, and λ is the wavelength of absorbed peak. The band gap energy of the samples corresponding to the absorption edge is found to be 3.41 eV for the PEG capped ZnO and 3.7 eV for CTAB capped ZnO nanoparticles.

3.2. Functional groups analysis

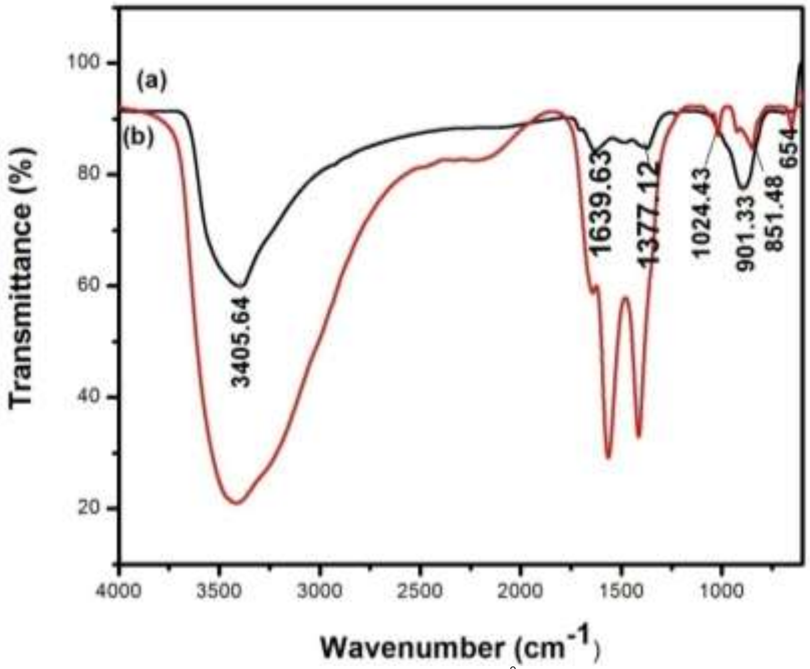

Fig 2.FTIR spectra of Zno nanoparticles calcinated at 400 °C (a) PEG and (b) CTAB capped ZnO

Figure 2. shows the presence of various functional groups due to the formation of PEG and CTAB capped ZnO are determined by FTIR spectra. The broad absorption peak at 3405cm^{-1} is attributed to stretching vibration of O-H group [13]. The peak appears at, 1574, 1639 and 901cm^{-1} are due to H-O-H bending vibration and it is assigned to water absorption on metal surface of the ZnO nanoparticles[14]. The peak at 1377 cm^{-1} is due to C-H bending of ZnO nanoparticles. The peaks appear at 851 cm^{-1} is assigned to stretching vibration of Zn-O[15] and the peak appears at 654 cm^{-1} is assigned to secondary vibration of the Zn-O nanoparticles.

3.3. Structural analysis

Figure 3. shows the powder XRD patterns of prepared zinc oxide nanoparticles using different capping agents by co-precipitation method. In each of these patterns seven reflections from (100),(022),(101),(102),(110),(103) and (112) planes are observed indicating the hexagonal structure with lattice parameters a=5.2835 A° b=5.2835 A° and c=14.09 A°. From this data, it is found that change in the capping molecule do not have any effect on the crystal structure of nanoparticles. The broad diffraction peaks are attributed to the characteristic small particle effect. All these diffraction peaks were perfectly indexed to the hexagonal structure corresponding to JCPDS (Card N0: 89-1397). The average sizes of ZnO nanoparticles for different capping agents are calculated using Debye-Scherrer formula,

$$D=0.89\lambda/\beta\cos\theta$$

Where 0.89 is Scherer's constant, λ is the wavelength of X-rays, θ is the Bragg diffraction angle and β is the full width at half-maximum (FWHM) of the diffraction peak corresponding to plane. The crystallite sizes are calculated using Scherer's formula is found to be around 24 nm and 22 nm for zinc oxide nanoparticle with PEG and CTAB capping agents respectively.

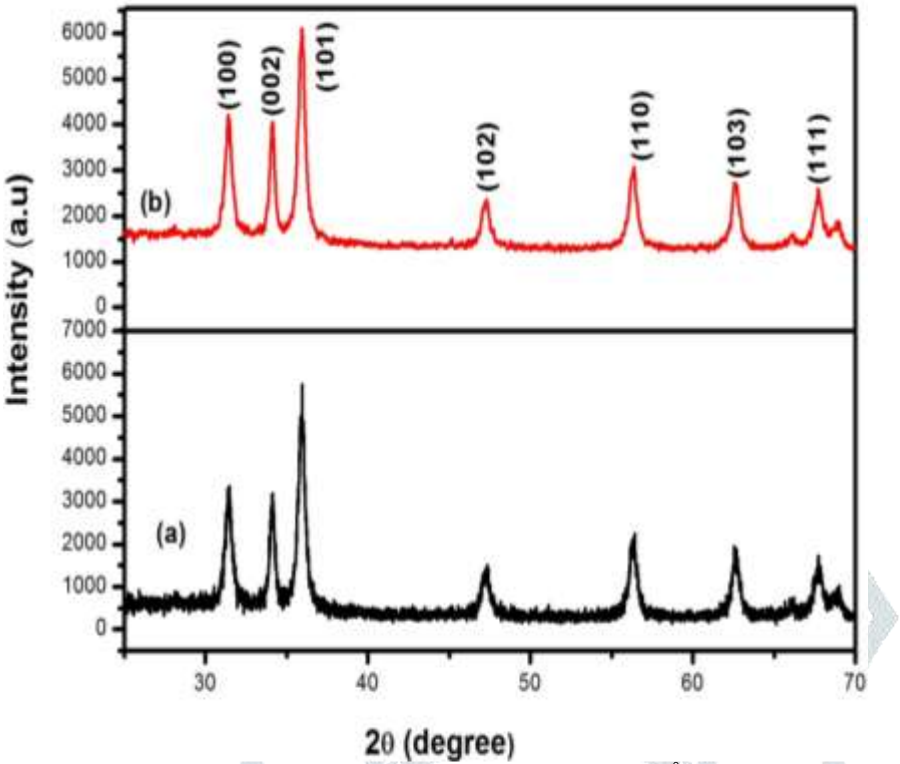

Fig 3. XRD Patteren of Zno nanoparticles calcinated at 400 °C (a) PEG (b) CTAB capped ZnO

3.4. Morphological analysis

Figure 4. shows the surface morphology of ZnO nanoparticles with different capping agents were investigated using Field Emission Scanning Electron Microscope (FESEM). The PEG capped ZnO calcinated at 400°C has nearly spherical in shape and from the figure it is clear that some of the particles are agglomerated. The CTAB capped ZnO calcinated at 400°C has clear spherical shape and the particles are distributed well. Therefore capping agents has important role on the morphological properties of metal oxide nanoparticles.

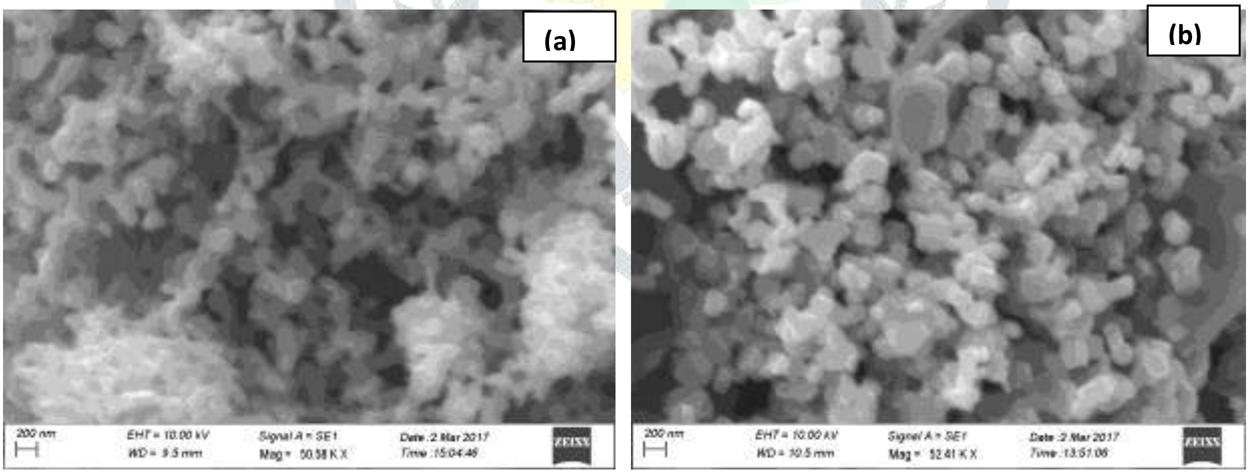

Fig. 4.FESEM images of (a) PEG (b) CTAB capped ZnO nanoparticles

4. Conclusions

PEG and CTAB capped ZnO nanoparticles are prepared by co-precipitation method and calcinated at 400°C. The powder X-ray diffraction patterns exhibit hexagonal structure for both synthesized PEG and CTAB capped ZnO nanoparticles. The crystallite size is found to be around 24 nm and 22 nm for zinc oxide nanoparticle with PEG and CTAB capping agents respectively. The absorped SPR peaks are blue shifted and centred at 364 nm for PEG capped ZnO and 340 nm for CTAB capped ZnO by UV-Visible spectra. The FESEM images of the prepared samples indicate that the PEG capped ZnO has spherical in shape and also CTAB capped ZnO nanoparticles have fine spherical shape. The formation of ZnO compound and presence of different functional groups are confirmed by FTIR analyses.

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