INTERNATIONAL JOURNAL OF RESEARCHES IN BIOSCIENCES, AGRICULTURE & TECHNOLOGY
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www.vmsindia.org

Structural and optical properties of CdO Nanomaterial synthesized by Autoclave combustion method

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Abstract:
Nano-sized cadmium oxide was synthesized by a simple autoclave combustion method using CdCl2.H2O as a metal precursor in the presence of polyethylene glycol and urea. The optical property of CdO nanoparticle was characterized by using UV-Vis Spectroscopy and structural property was studied using FTIR and XRD. The XRD shows the formation of rocksalt structure of CdO nanoparticle while FTIR shows existence of Cd-O bond.
Keywords: Autoclave method, XRD, rocksalt structure, band gap.

Introduction:

Cadmium oxide is an inorganic compound with the chemical formula CdO. It crystallizes in cubic rocksalt lattice with anion centers and octahedral cation. It occurs naturally in the rare mineral monteponite. It can be found as brown or red crystals or colourless amorphous powder. It is an n-type semiconductor obtained by burning elemental cadmium in air with the band gap in the range of 2.2–2.8 eV and possesseslow resistivity (10^{-2} to 10^{-4} Scm^{-1})due to the defect of oxygenvacancies and cadmium interstitials[1-3]. Cadmium oxide (CdO) has high electrical conductivityand high optical transmittance with a moderate refractiveindex in the visible region of the solar spectrum.CdO films havebeen successfully used for many applications, including usein gas-sensing devices, photodiodes, transparent electrodes,phototransistors, and photovoltaic solar cells[4]. Further, the CdO films are used in liquefied petroleum gassensor; the sensitivity and electrical conductance of the films arereproducible[5]. CdO has not only the unique optical and optoelectrical characteristics but also has the selective catalytic properties that can be used to photo degrade some of the organic compounds, dyes, pigments and many of environmental pollutants[6-8].

Zouet al.[9] has prepared CdO nanoparticles by the micro-emulsion method employing AOT reverse micelles. There is also a report of stearate coated CdO nanoparticles of 5–10 nm size range, obtained by the micro-emulsion method starting from an aqueous solution of a cadmium salt and stearic acid in xylene[10]. Wu et al.[11] prepared a nanometer-sized CdO organosol from an aqueous solution of Cd $(NO_3)_2$, in the presence of a surfactant and toluene as solvent.

In this work, CdO nanomaterial has been synthesized by autoclave combustion method with cadmium chloride and polyethylene glycol as raw material at heat treatment pressure of 110 atm. for 1 hourwhich is very simple and economical method. The product wascharacterized by XRD, UV-Vis spectroscopy and FT-IR techniques.

Materials and methods:

The chemicals Cadmium chloride, Ethylene glycol and urea used in the preparation were of analytical reagent grade purchased from S-D fine lab, INDIA.The crystal structure wasstudied by a Brucker D8 advance X-ray Diffractometer at UGC-DAE Consortium, Indore with Cu K radiation (λ = 1.54 Å) to check the phase system and purity of the sample.The infrared spectrum of the solid nanoparticle was recorded by Shimazdu FT-IR Spectrometerwhile optical study was performed using Shimazdu 1800 double-beam UV–visible spectrophotometer in the range of 200-800 nm at Kamla Nehru college, Nagpur.

Preparation methods:

The synthesis has been done by hydrothermal methods. 30 ml of ethylene glycol used as a stabilizer and 50ml of 1M cadmium chloride was stirred for 30 minutes. To this solution 1M of urea was added. The solution turns milky white after addition of urea. The reaction mixture was kept for 1 hrs. in autoclave. After autoclaving the system, the white precipitate of the CdO formed. The synthesized compound so obtained was then washed with distilled water three times and then finally with alcohol. The precipitate was then dried in oven

at 150°C for 5 hours. This product were then used for characterization.

Results and Discussion:

1. XRD:

Fig. 1 shows the XRD pattern of CdO nanoparticle. All the diffraction peaks can be well indexed to the cubic crystalline phase of the CdO nanomaterial, with lattice constants of a=2.734Å. The results indicate that the samples consist of pure phase and are crystalline in nature.The XRD peaks of CdO can be found to (012), (110), (111), (200) and (220) at a diffracting planes at 2θ = 23.53°, 29.48°, 30.32°, 38.74° and 53.13° respectively (JCPDS 65-2908). The particle size of nanomaterial was calculated using the Debye-Scherer equation:

$$D = \frac{k\lambda}{\beta \cos\theta}$$

Where K is a constant equal to 0·89,

λis the X-ray wavelength (0·154095 nm),

βis the full wavelength at half maximum and θ the half diffraction angle.

The grain size calculated using the relative intensity peak (111) for CdO nanoparticles was found to be 65 nm.

2. FTIR:

Fig. 2 shows the IR spectra for the sample product CdO nanoparticle. IR spectra shows four characteristic absorption peaks at 3518 cm^{-1}, 3468 cm^{-1}, 3354 cm^{-1} and 3199 cm^{-1} which are attributed to the υ_{as}(N-H) antisymmetrical and υ_{s}(N-H) symmetrical stretching vibrations, respectively, and also can be assigned to $\upsilon_{(OH)}$ stretching vibration of water absorbed from the surrounding. The overlapping of –OH bands of H_2O molecule to the vibration bands of NH_2 molecule can results in the broadening of the bands. The other peak at 1793-1365 cm^{-1} corresponds to the $\upsilon_{(C=O)}$ and $\upsilon_{(O-C-O)}$ stretching vibrations of the carbonyl group. However, the FTIR peaks at 420cm^{-1}indicates the confirmation of CdObond[12].

3. UV-Vis spectroscopy:

UV– visible absorption of synthesized Cadmium oxide colloidal solution illustrates a wide absorption peak centered at 330 nm with a long tail as shown in Fig. 3.The band gap of semiconductor materials increases with the decrease in particles size, which leads to the shift of the absorption edge toward high energy; this is the so-called quantum size effect The absorption band of the CdO nanoparticles have been shows a blue shift due to the quantum confinement of the exactions present in the sample compare with bulk CdO particles. This optical phenomenon indicates that these nanoparticles show the quantum size effect. The peak observed at 390 nmcorresponds to the band-edge emission of the CdO nanocrystals[13]. The maximum absorption of the nanoparticles shows at 330nm and band gap energy was calculated to be 3.75eV. The optical band gap, (Eg) of the samples are determined from the Tauc equation.

$$(Ahv)^n = B\left(hv - E_g\right)$$

wherehυ, A, B andn are photo energy, absorbance,constant relative to the material and n = ½ or 2 for indirect transition and direct transition, respectively.

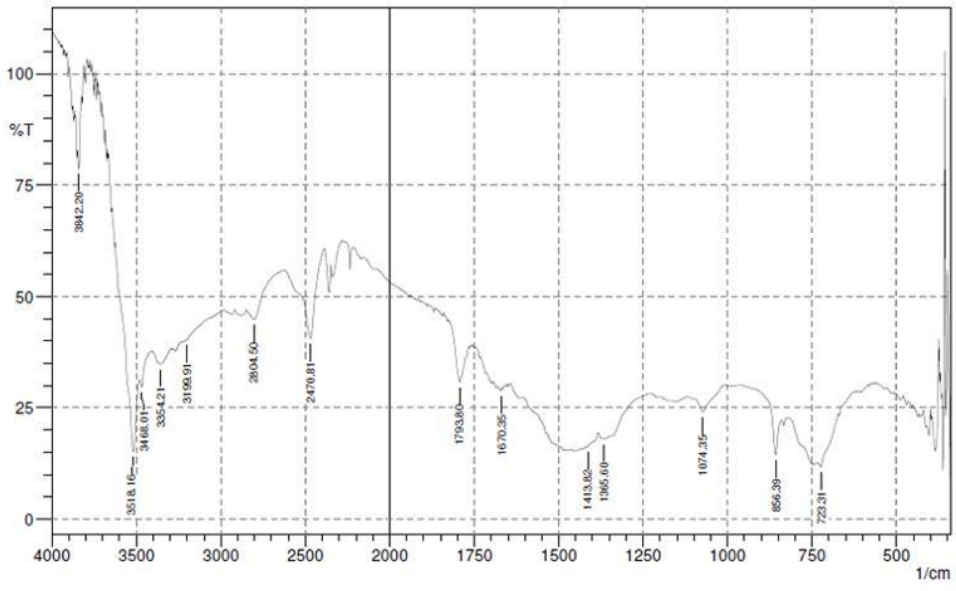

Fig. 2 FTIR spectra for CdO nanoparticles

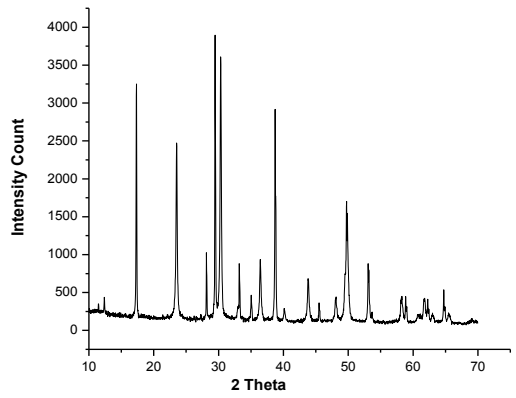

Fig. 1 XRD pattern for Cadmium oxide nanoparticle

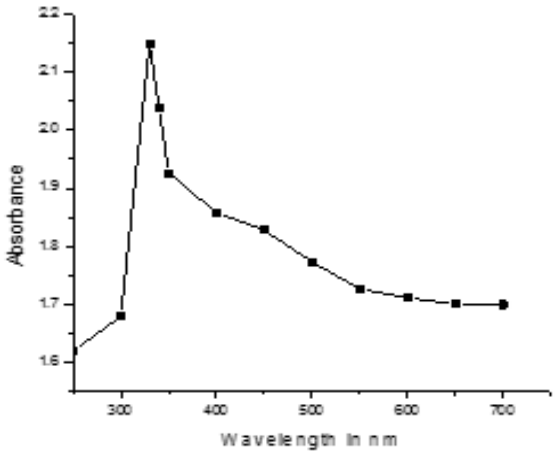

Fig. 3. UV-Vis absorption spectrum of CdO nanoparticle

Conclusion:

CdO nanoparticles has been synthesized by autoclave combustion method using very easy, cheap and convenient process. The XRD study has shown the formation of rocksalt crystal structure. FTIR and UV-Visible spectroscopy shows the existence of CdO nanoparticles.

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