EFFECT OF THE CAPPING AGENT ON THE OPTICAL ABSORPTION EDGE OF COPPER OXIDE NANOPARTICLES FILM

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Abstract

In this work, the capped and uncapped copper oxide (CuO) nanoparticles film with an average size ranging from 8.7 - 6.2 nm have been prepared by a chemical wet procedure using copper (II) sulfate with sodium hydroxide at 50 °C. The EDTA was used as a capping agent and the obtained samples were investigated by UV visible spectrum. The uncapped and EDTA capped CuO nanoparticles reveals two bands observed at 310 nm and 232 nm for uncapped and EDTA capped CuO nanoparticles respectively. The optical absorption spectra exhibits the energy band gap for uncapped and EDTA capped (CuO) in the range of (3.8 - 4.5) eV respectively.

Keywords: Optical band gap, CuO nanoparticles, capping agent.

Introduction

Nanoparticles of metal oxide have attracted the amount of attention over recent years, because of the distinction of their physical and chemical properties. Among all other metal oxides, Copper oxide (CuO) is a material that possesses scientific and industrial applications (Jolivet, 2000) in the areas of magnetic storage media and photonic devices (Mishina et al.,2001; Cao et al.,2008) due to, their unique properties like superconductors and photovoltaic properties. (Frietsch et al.,2000; Sukhorukov et al.,1998; Carnes and Klabunde,2003).

CuO is a p-type semiconductor oxide, with a narrow indirect band gap of ~1.21 eV, and high absorption properties that make it a promising for solar cell fabrication (Xia et al.,2014; Masudy et al.,2013; Kumar et al.,2013). Efforts of researchers have been made for synthesizing CuO nanoparticles by using different methods such as thermal decomposition (Darezereshki and Bakhtiari,2011), sol-gel (Hong et al.,2002), chemical precipitation (Tran and Nguyen,2014). as well as electrochemical methods (Son et al., 2009; Poizot et al., 2003 and Yuan et al., 2007) in which various nano morphologies can be acquired.

Nanoparticles in the way of films can be utilized for solar energy. Therefore, it is considered desirable to develop the method to synthesize high-quality thin film of CuO nanoparticles for device fabrication. In this paper, reacting CuSO4.5H2O as the source of Cu and an aqueous
NaOH solution in the presence of EDTA as a capping agent, we could obtain film of CuO nanoparticles at the interface.

**Experimental section**

**Chemical reagents**

Copper (II) sulfate pentahydrate and sodium hydroxide pellets obtained from T-Baker Lab Chemicals, India, EDTA and toluene from BDH chemicals Ltd Poole, England

**Synthesis of CuO nanoparticles**

50 ml (0.437 g) copper (II) sulfate pentahydrate as the Cu source in 20 ml of toluene was taken in a beaker and 20 ml of an aqueous solution containing 1.2 g of NaOH was slowly injected into the beaker was placed inside oven left undisturbed at 50 °C for 8 h.

\[
\text{CuSO}_4 \cdot 5\text{H}_2\text{O} + 2\text{NaOH} \rightarrow \text{Na}_2\text{SO}_4 + \text{Cu(OH)}_2 + 5\text{H}_2\text{O}
\]

\[
\text{Cu(OH)}_2 \rightarrow \text{CuO + H}_2\text{O}
\]

The achievement of the reaction was indicated by the appearance of black colour at the interface as shown in figure1. Reactions were similarly carried out by using 0.002 mM of 10 ml EDTA as a capping agent, which added to NaOH and injected to the bottom of the beaker.

![Figure 1: Photographs Show the Preparation of CuO Film of Nanoparticles](image)

The interfacial film of uncapped and EDTA capped CuO nanoparticles were dissolved in ethanol and quartz cell were used for the measurements. The as-prepared CuO nanoparticle thin films were analyzed by CE7400-7000 3ERIES Double Beam UV-vis spectrophotometer manufacture Buck scientific, Inc. The scan distance range was between 200-800 nm. The absorption spectra were recorded at room temperature. In this study, a simple UV-vis was
utilized to calculate the bandgap energy using the Tauc relation (Tauc and Editor,1974; Litton and Reynolds,1964; Manjunath, 2016).

\[(\alpha h\nu) = A (h\nu - E_g)^n\]

Here, \(E_g\) is bandgap, \(A\) is constant related to the material, \(\alpha\) is absorption coefficient, \(h\nu\) is photon energy, \(n\) is 2 for direct transition or 1/2 for an indirect transition.

**Result and dissection**

The UV-vis spectrum of the uncapped and EDTA capped copper oxide nanoparticles exhibits absorption peaks centered at 310 nm and 232 nm (figure 2). It reveals the peak position and the maximum absorption (\(\lambda_{max}\)) blue-shifted from 310 nm in uncapped CuO nanoparticles to 232 nm in EDTA capped CuO because of direct transition of electrons from the valence band to the conduction band as well as quantum confinement effect which occurs when particles size becomes as good as with or less than exciton Bohr radius. (Yin et al., 2005; Rahdar.,2015; Sawsan et al.,2014).

![Figure 2: Absorption Spectra of Film Copper Oxide (a) Uncapped CuO Nanoparticles, (b) EDTA Capped CuO of Nanoparticles.](image)

The absorbance against wavelength plots was changed to tauc plot and band gap energy was calculated by using tauc's equation by plotting \((\alpha h\nu)^2\) against \(h\nu\) (figure3). The extrapolation straight line is obtained for all prepared samples gives the value of the absorption edge. The calculated band gap values of CuO nanoparticles are 3.8 ev in uncapped and 4.5 ev in EDTA capped CuO nanoparticles. Both the values are higher than the recorded value bulk (1.21 ev) This redshift in energy band gap due to size reduction and the quantum confinement effect (Siddique et al., 2014; Loubaba et al., 2018; Yuan et al., 2019).
The particles size that estimated from UV absorption spectra using the formula below was in the range of 8.7 nm in uncapped CuO and 6.2 nm in EDTA capped CuO (Phoka et al., 2009; Purushottam et al., 2016).

\[ E_g = E_{\text{bulk}} + \frac{\hbar \pi}{2R \left( \frac{1}{m_e} + \frac{1}{m_h} \right)} - 1.8e^2/\varepsilon R \]

\( E_g \) is band gap energy of the nanoparticle, which will be determined from the UV-Visible absorbance spectrum, \( E_{\text{bulk}} \) for CuO nanoparticles which is 1.21 ev, \( \hbar \) is Planck’s Constant, \( R \) nanoparticles size, \( m_h \) and \( m_e \) are effective mass for electrons and hole, \( e = 1.602 \times 10^{-19} C \), \( \varepsilon \) is dielectric constant.

**Conclusion**

The CuO nanoparticles were successfully created by a facile method at comparatively low temperature. The optical band gap of CuO nanoparticles was found to be larger than the bulk band gap value (1.21 eV) as expected due to the nano size of the particles. This work can lead to the synthesis of various mixed metal oxides for applications for solar energy or supercapacitors.

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References


