



Extraction of important electrical parameters of CuO

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ARTICLE INFO

Article history:

Received 23 July 2010

Accepted 14 November 2010

Keywords:

CuO

Dip coating technique

Electrical parameters

Compensation ratio

ABSTRACT

Conductivity, X-ray diffraction (XRD), optical absorption and atomic force microscopy (AFM) measurements of CuO thin film were presented. Three distinct electrical conduction contributions with discrete characteristic activation energies were observed. The applicability of various theoretical models was considered to explain results on electrical transport. We extracted important electrical parameters of CuO, which might be useful for its gas sensor applications.

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1. Introduction

There is a growing interest in the development of transition metal oxides in the literature of recent years. Especially, electrical properties of these materials have been studied extensively [1–5]. CuO is a p-type transition metal oxides semiconductor [6]. It has received considerable attention due to its great potential as a material for gas sensor applications [7–9].

Although the grain boundary (GB) transport properties give rise to important information on gas sensing properties, determination of the presence of different conduction mechanisms in CuO is still debatable. Therefore, understanding the charge transport can be important to improve sensitivity properties. One of the most important parameters related to the performance of gas sensors is the surface trap density (N_t) determining the Debye screening length (L_D) of the material. The data on the electrical parameter related to gas sensing properties should be provided to improve gas sensitivity. Decreasing N_t in transitional metal oxides is an effective way to enhance gas sensitivity. When L_D is about half the crystallite size (L), maximum sensitivity can be achieved [10]. The optimum sensitivity is obtained for small L , large L_D and relative low carrier concentration [10].

In this work, we aim at demonstrating the determination of electrical transport properties by processing the temperature dependence of conductivity of polycrystalline CuO, which might also help to interpret important electrical parameters for its gas sensor applications.

2. Experimental

In this work the starting solution for the deposition of copper oxide was prepared by dissolving copper acetate [$\text{Cu}(\text{CH}_3\text{COO})_2 \cdot \text{H}_2\text{O}$] in ethanol. Afterwards lactic acid and triethylamine ($\text{C}_6\text{H}_{15}\text{N}$) were added to the resulting solution. The films were deposited by dip coating technique on glass substrates that were ultrasonically cleaned in de-ionized water and acetone (CH_3COCH_3 , Merck) for 30 min. Film deposition was carried out in air at room temperature with a controlled speed of approximately 0.36 cm/s. After withdrawal, the substrate with the liquid film adhering to it is baked at 300 °C for 5 min in air. The above coating and baking processes were repeated to increase the thickness of the film. Finally the as-deposited films were annealed in air at 500 °C for 1 h.

The microstructure of the deposited films was investigated using an Inel-EQUINOX 1000 diffractometer. The radiation source, the wavelength and the scanning range 2θ of the diffractometer were CoK_{α} , 0.179 nm and 30–65°, respectively. The optical band gap of the films was calculated by means of UV–vis–NIR transmittance measurements performed by Shimadzu UV-3600 spectrophotometer in the spectral range 300–1500 nm.

The surface morphology of the films was also observed by a SPM Solver-PRO (NT-MDT) in semi-contact mode. The root-mean-square (RMS) values of surface roughness were estimated. The electrical conductivity measurements were carried out using Keithley 2420 programmable constant current source in a temperature range 125–365 K.

3. Results and discussion

The X-ray diffraction patterns for CuO film are shown in Fig. 1. The spectra show the well-resolved two diffraction peaks.

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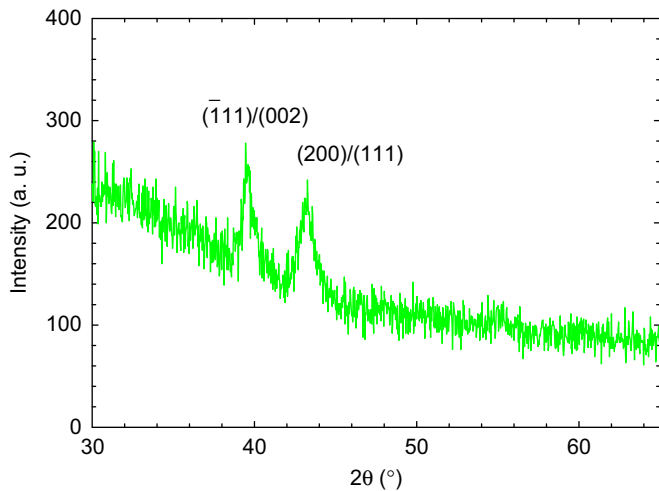
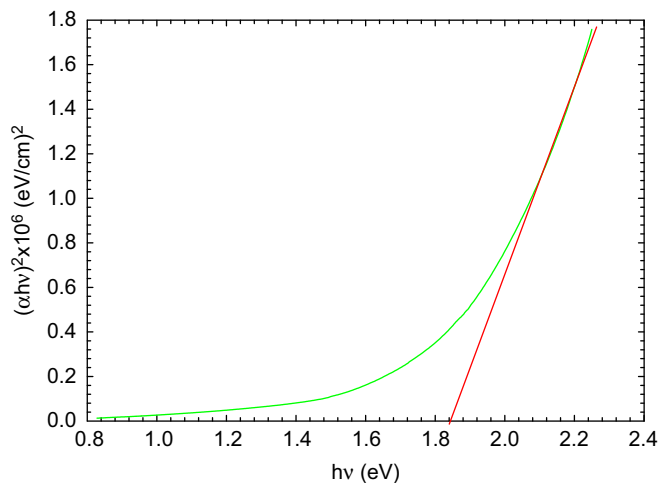


Fig. 1. XRD spectra of CuO.

Fig. 2. Plot of $(\alpha hv)^2$ vs. $h\nu$ for CuO.

These peaks correspond to the reflection of the $(111)/(002)$ and $(200)/(111)$ planes of standard JCPDS data card of CuO [11]. Since all the peaks are sharp, it is evident that the films are polycrystalline in structure. The crystallite size for crystallites with $(200)/(111)$ plane was calculated using Scherrer's formula, neglecting peak broadening due to residual stresses in the films, $L = 0.9\lambda/(\beta \cos \theta)$ where β is the broadening of diffraction line measured at half its maximum intensity in radians and λ is the wavelength of X-rays (0.179 nm). The calculated value of L is 14.9 nm.

The optical band gap of the film has been determined on the basis of UV–vis transmission measurements. For this, the fundamental absorption coefficient (α) was evaluated using $\alpha = (\ln T^{-1})/t$, where t is the film thickness and T is the transmittance. The value of absorption coefficient is of the order of 10^4 cm^{-1} supporting the direct band gap nature of the material. The nature of the direct allowed transition is determined using the relation

$$\alpha h\nu = A(h\nu - E_g)^{1/2} \quad (1)$$

where $h\nu$ is the photon energy, E_g is the optical band gap energy and A is a constant. The typical plot of $(\alpha h\nu)^2$ vs. $h\nu$ is depicted in Fig. 2, which indicates the presence of direct transition. The linear portion is extrapolated to $\alpha = 0$ on the energy axis, which gives the band gap energy of 1.82 eV for the sample. It has been reported that the band gap of CuO can be changed to a wide range (1.75–2.15 eV) depending on the preparation conditions of CuO [12–15].

The surface morphology of the films is shown to be three- (3D) and two-dimensions (2D) in Fig. 3. AFM analysis showed that films are polycrystalline and have nano-grains. The root-mean-square (RMS) value of surface roughness was estimated as 4.04 nm.

In order to get a deeper insight into the conduction mechanisms, the temperature-dependent conductivity characteristics were performed in a temperature range of 125–365 K for the investigated sample. Fig. 4 shows the Arrhenius plot of the conductivity, σ , over whole temperature range. In particular, it is observable that no single law conduction can fit the entire curve of conductivity. The conductivity curve can be divided experimentally by operating in appropriately three regions, i.e. (i) $\Delta T_1 = 365\text{--}295 \text{ K}$, (ii) $\Delta T_2 = 295\text{--}200 \text{ K}$ and (iii) $\Delta T_3 = 200\text{--}125 \text{ K}$ denoted by 'high temperatures', 'intermediate temperatures' and 'low temperatures', respectively.

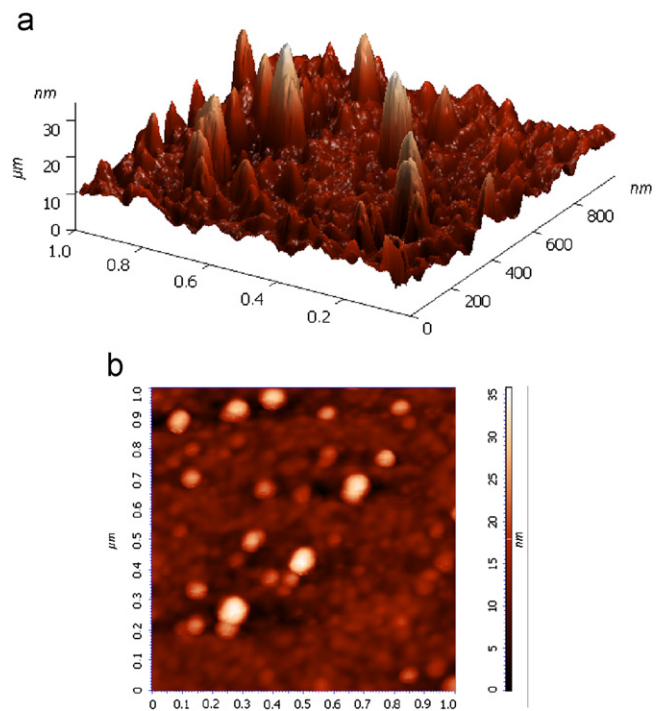
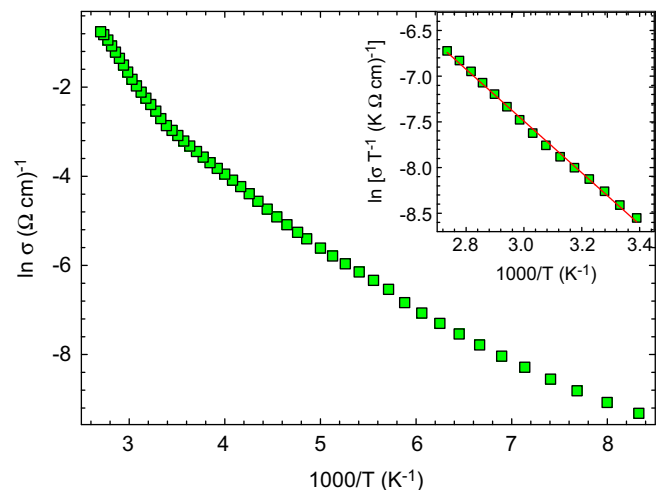


Fig. 3. (a) Three-dimensional (3D) and (b) two-dimensional (2D) AFM images of CuO.

Fig. 4. Temperature dependence of conductivity plotted as $\ln(\sigma)$ vs. $10^3/T$ in a temperature range 125–365 K. Inset represents conductivity plotted as $\ln(\sigma T^{-1})$ vs. $10^3/T$. Solid lines are the best-fit lines with Eq. (2).

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