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ความสัมพันธ์ระหว่างผงซิงค์ออกไซด์ที่สังเคราะห์ที่อุณหภูมิต่างๆ กับสมบัติทางแสง

CORRELATION BETWEEN NANOCRYSTALLINE ZnO POWDERS SYNTHESIZED AT DIFFERENT REACTION TEMPERATURES AND OPTICAL PROPERTIES

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บทคัดย่อ: ผง ZnO ที่มีขนาดผลึกในระดับนาโนเมตรถูกเตรียมด้วยวิธีการตกตะกอนจากสารตั้งต้น $Zn(CH_3COO)_2.2H_2O$ และ NaOH ผง ZnO ที่เตรียมได้มีโครงสร้างแบบเวอร์ตไซท์ที่มีขนาดผลึก 30, 32 และ 35 nm เมื่อสังเคราะห์ที่อุณหภูมิ 25, 60 และ 80 °C เป็นเวลา 1 ชั่วโมง ตามลำดับ ผง ZnO ที่เตรียมได้ทั้งหมดแสดงการส่องผ่านแสงมากกว่า 90%ในช่วงวิสิเบิลและแสดงค่าช่องว่างพลังงานขนาด 3.24 eV

Abstract: The nanocrystalline ZnO powders were prepared by precipitation method using $Zn(CH_3COO)_2.2H_2O$ and NaOH as precursors. The prepared nanocrystalline ZnO powders indexed the wurtzite structure with the crystallite size of about 30, 32 and 35 nm when synthesizing at 25, 60 and 80 °C for 1 hour, respectively. All nanocrystalline ZnO powders performed the high transmittance over 90% in the visible region with the band gap of 3.24 eV.

Introduction: As far as nanomaterials are concerned, ZnO is one of the candidates for electronic and optic devices. ZnO normally forms hexagonal or wurtzite structure. The lack of center of symmetry combining with a large electromechanical coupling, results in strong piezoelectric and pyroelectric properties and the consequent use of ZnO in mechanical actuators, piezoelectric sensors and surface wave acoustic devices [1,2,3,4]. Moreover, ZnO that has a wide band gap of about 3.3 eV and large exciton binding energy of 60 meV at room temperature is an important candidate for room temperature UV lasers and short-wavelength optoelectronic devices [5,6]. Recently, there has been a great growing interest in the synthesis of nanocrystalline ZnO powders by chemical route. So, we investigated the formation of nanocrystalline ZnO powder at various reaction temperatures and we also studied the structural and optical properties of nanocrystalline ZnO powders.

Methodology: All the chemical reagents used in this experiment were analytical grade and were used without further purification. In a typical procedure, 4.3898 g $Zn(CH_3COO_2).2H_2O$ was first dissolved in 100 mL distilled water with continuous stirring until a homogeneous solution was obtained. Later on, 3.2627 g NaOH that was dissolved in 100 mL distilled water was slowly added to zinc precursor solution.

The white precipitates were achieved and were each vigorously stirred at 25, 60 and 80 °C for 1 hour before filtering, rinsing with distilled water, drying at 60 °C and calcining at 500 °C for 1.5 hour. The phase identifications of the calcined powders were examined by powder X-ray diffractometer (XRD, X'Pert MPD, Philips) with CuK_α radiation (λ = 0.15406 nm). The shape and grain size of the calcined powders were evaluated with scanning electron microscopy (SEM, JSM-5800 LV, JOEL) and the optical spectra were measured in the range of 200-800 nm with a UV-VIS spectrophotometer (UV-2401, Shimadzu).

Results, Discussion and Conclusion: Reaction temperature is an important parameter to control the morphology of ZnO powder. So, we investigated the effect of reaction temperatures at 25, 60 and 80 °C that affected on the crystal structure as depicted in figure 1.

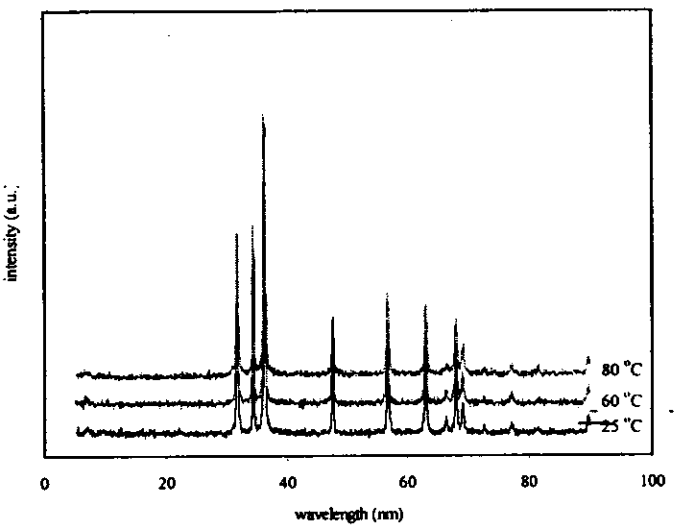

Figure 1. The XRD patterns of ZnO powders prepared at 25, 60 and 80 °C for 1 h

The XRD patterns of all samples indexed the wurtzite or hexagonal structure in correspondence with the JCPDS (card number 36-1451). The crystallite size was estimated by Scherrer's formula; $D = \frac{k\lambda}{\beta \cos\theta}$ where D is the crystallite size, k is the constant, λ is the wavelength of x-ray used, β is the line width in radian at half maximum intensity and θ is the Bragg angle [7]. It is obvious that the crystallite size increased with increasing the reaction temperature as depicted in figure 2.

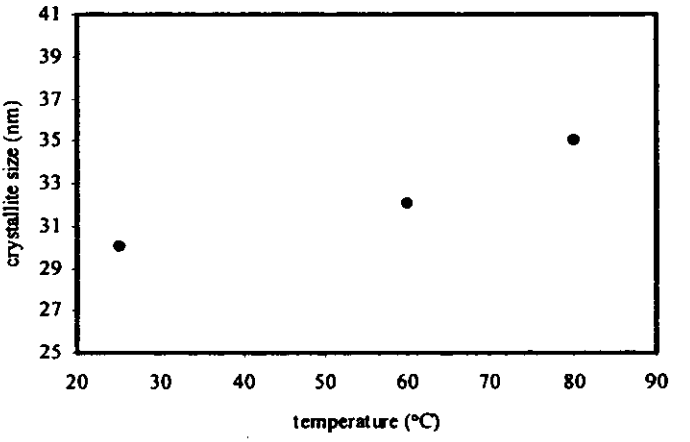

Figure 2. Dependence of crystallite size on reaction temperature

The high transmission in visible region is very important in many applications. In this study, it is obvious that the nanocrystalline ZnO powders performed in a highly transparent mode in visible region as shown in figure 3.

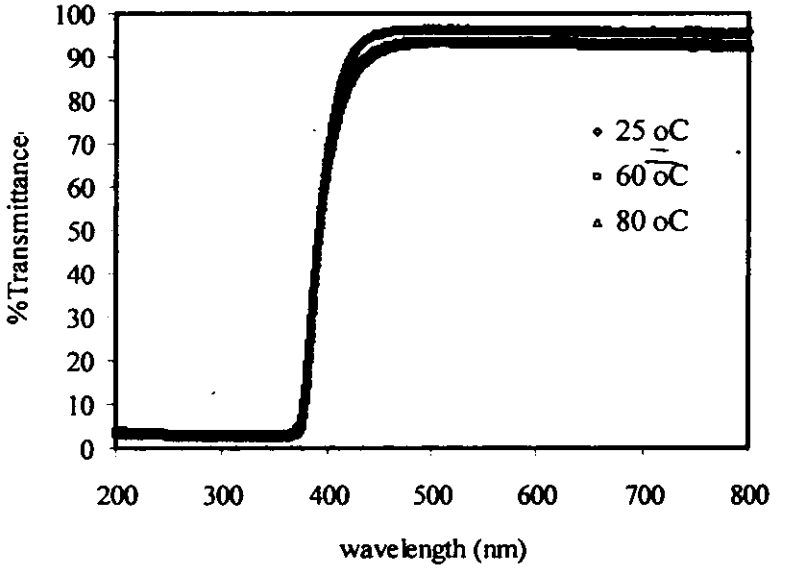

Figure 3. Room temperature optical transmittance spectra of ZnO powders prepared at different reaction temperatures.

Based on the transmittance spectra, we can estimate the band gap of nanocrystalline ZnO powders from the relationship; $(\alpha h\nu)^2 = E_D(h\nu - E_g)$ where α is the optical absorption coefficient, $h\nu$ is the photon energy, E_g is the direct band gap and E_D is the constant [8].

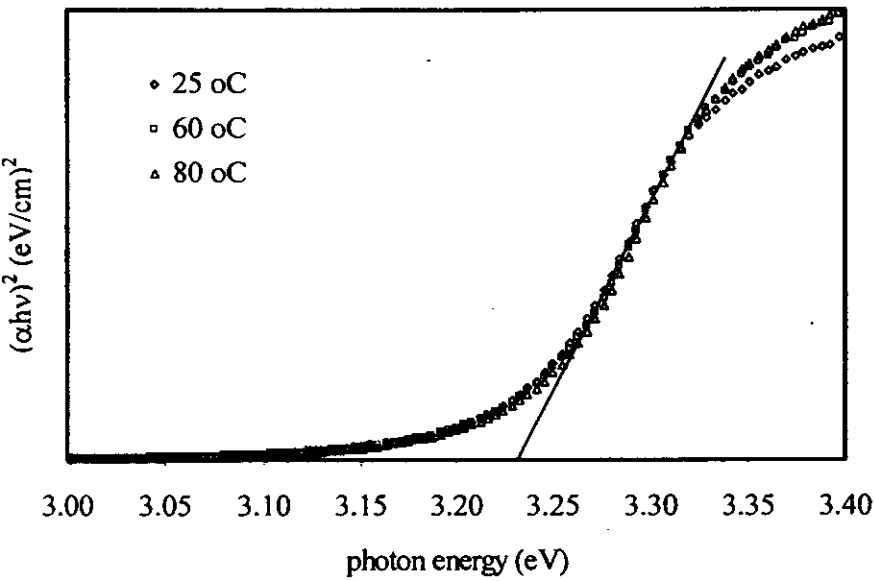

Figure 4. Evolution of the $(\alpha hv)^2$ vs. hv curves of nanocrystalline ZnO powders prepared at different reaction temperatures.

Figure 4 shows a graph of $(\alpha hv)^2$ vs. hv for nanocrystalline ZnO powders. The linear portion of the curves when extrapolating to zero was an optical band gap value of nanocrystalline ZnO powders. In this study, we obtained the optical band gap of about 3.24 eV for all nanocrytalline ZnO powders.

The nanocrystalline ZnO powders with the smallest crystallite size of about 30 nm was successfully synthesized at reaction temperature of 25 °C by simple precipitation method using $Zn(CH_3COO)_2.2H_2O$ and NaOH as starting materials. The optical band gap of all ZnO powders is about 3.24 eV.

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