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The effect of milling time on structural, optical and photoluminescence properties of ZnO nanocrystals

A.A. Othman*, M.A. Osman, A.G. Abd-Elrahim

Physics Department, Faculty of Science, Assiut University, Assiut 71515, Egypt

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ABSTRACT

The crystallite size of commercial ZnO nanocrystals was tuned from 22.5 to 13.8 nm by ball-milling technique. X-ray diffraction patterns of mechanically milled ZnO nanocrystals reveal that milled samples possess the wurtzite-type hexagonal structure of ZnO. Increasing milling time results in the decrease of crystallite size and reduction of lattice parameters due to a slight increase of internal compressive strain and dislocation density. Scanning electron microscope images demonstrate the appearance of large agglomerated particles with ambiguous edges due to large aggregation tendency with slight variation in the particle size at milling time 8 h. Analysis of the optical absorption spectra at different milling time indicates the blue shift of exciton absorption peak and optical gap photoluminescence spectra reveal that mechanical milling of ZnO NCs leads to quenching of emission intensity due to the creation of nonradiative centers via increasing thermal strain and mechanical deformation produced during the milling process.

1. Introduction

Ball milling technique is a room temperature promising technique for large mass production of nanostructured materials that used in many important applications because safety, economic consumption of energy [1]. Structural and interfacial properties of nanomaterials such as a crystallite size, orientation, and morphology, defects, lattice strain strongly affect its optical absorption and photoluminescence characteristics. The need for mass production of desirable size-dependent optical and optoelectronic properties for technological applications with reasonable low cost, make the mechanical milling preferable method for obtaining various nanostructured materials such as ZnO. An N-type semiconductor such as ZnO with a large band gap of 3.3 eV and high exciton binding energy of 60 meV [2], has unique properties such as low cost, non-toxicity, abundance in nature, suitability for doping [3] as well as the high thermal and chemical stability. This makes ZnO extensively used in many applications such as gas sensors [3], solar cells [4], luminescent materials [5], light emitting devices [6], UV photodetectors [7], piezoelectric devices [8], spintronics [9], and cancer treatment [10]. Moreover, ZnO nanostructures revealed dramatic changes in their structural, electronic and optical properties compared to those of their bulk [11,12]. It is well known that lowering of grain size enhances the grain-surface region in the material. Such regions are rich by defect [13] and the nature and abundance of these defect centers play a crucial role in controlling the physical properties of ZnO [14,15].

* Corresponding author.
E-mail address: aaelho@yahoo.com (A.A. Othman).

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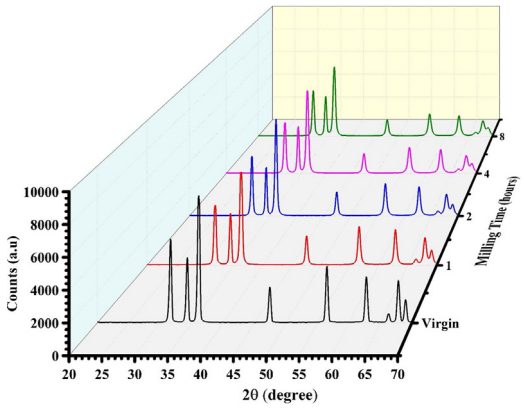

Fig. 1. XRD patterns of ZnO nanocrystals at different milling time.

Dutta et al. [16] have studied the effect of milling energy on the optical absorption and structure properties of ball milled ZnO nanocrystals. They found that increasing of milling time resulted in the increase of interfacial defects, which cause the evolution of new localized energy levels within the optical gap, the increase of localized tail states width and by the reduction of the measured optical band gap with increasing milling time; meanwhile Giri et al. [17] have found that the increase of milling time in ZnO nanoparticles resulted in the blue shift of the optical band gap accompanied by the reduction of photoluminescence emission intensity. They attributed this behavior to a combined effect of both weak quantum confinement and mechanical induced lattice strain. Qin et al. [18] have studied the strain-induced change in nanocrystalline materials lattice parameters and illustrated that the lattice strain induced by the deviations of atoms in the crystallites from their ideal sites near the grain boundaries and the change of lattice parameters are related to the grain size and the grain boundary structure.

In our previous work we have studied the effect of doping by Cu and Mn ions in ZnO host lattice prepared by ice-bath assisted sonochemical technique [19,20] and we found that the increase of lattice strain induced by foreign atoms (Cu or Mn) resulted in overall quenching of photoluminescence emission intensity due to the formation of nonradiative centers. On the other hand another, we have observed the quenching of photoluminescence emission of ZnO nanocrystal by thermal annealing [21]. Hence, for in the present for more understanding the role of surface and interfacial defects induced by mechanical milling energy on the structural and morphological changes, optical absorption and photoluminescence characteristics of commercial ZnO nanocrystals.

2. Material characterization

Mechanical milling for different milling times (1, 2, 4, 8 h) by a planetary ball mill (Fritsch Bulverisette version 6, GmbH, Duisburg, Germany), with zirconium oxide balls (approximately 10 mm in diameter) and bowls (500 ml) at ball to powder mass ratio 10 to 1 and 250 rpm has been carried out for milling of commercial ZnO purchased from Chem. lab nv company, Belgium (99.5% purity, 81.37 g/mol and density of 5.61 g/cm^3). Structural changes of ZnO nanopowder (NPs) at different milling time due to mechanical milling process were characterised by PW 1700 X-ray diffractometer (XRD) with Cu K_α radiation $\lambda = 0.154056$ nm at a diffraction angle (2θ) in the range 20–70° with a step of 0.06° and refined by crystal structure Celref Software. The surface morphology of the as-purchased and milled ZnO NCs was examined by scanning electron microscope (SEM) (Shimadzu Superscan SSX-550). Measurements of optical absorption and transmittance spectra were carried out using UV–vis Perkin-Elmer Lambda 750 spectrophotometer in the range 200–700 nm. Photoluminescence (PL) emission spectra were recorded by JASCO FP-6300 spectrofluorometer at excitation wavelengths 325 nm and the normalized spectra were deconvoluted by Origin Software to identify the exact peak position of the emission bands.

3. Results and discussion

3.1. Effect of milling time on the structural parameters of nanostructured ZnO

XRD patterns of the as-purchased and milled ZnO at various milling times were refined by crystal structure celref software for exact determination of the diffraction peaks angles (2θ), Fig. 1. It can be observed that the as-purchased and milled samples reveal pronounced diffraction peaks correspond to (100), (002), (101), (102), (110), (103), (200), (112) and (201) planes that in good match with the standard data of Wurtzite-type hexagonal structure of ZnO crystal with space group $P6_3mc$ (JCPDs card no: 04-008-8198). In addition, it can be observed that increasing milling time resulted in the decrease of diffraction peaks intensity, as well as the broadening of diffraction peaks due to milling induced structural defects and the accompanied