Influence of deposition time on structure and substructure of ZnO

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Summary

The methods of scanning electron microscopy, X-ray diffraction and Raman spectroscopy were used for investigation of structural features of ZnO films synthesized by chemical bath deposition from zinc nitrate and ammonia solution. X-ray and Raman studies revealed that the films are single phase and highly oriented along growth texture of [002]. Condensates have a hexagonal structure with lattice constants, of a = 0.32486 nm, c = 0.52087 nm. Coherent scattering domain size and level of microstrain were, respectively, L ~ 26 - 42 nm and ε ~ (0.59 - 3.09) 10^{-3} and determined by regimes of films obtaining.

Introduction

Owing to the large band gap (E_g = 3.37 eV) and large exciton binding energy at room temperature (~ 60 meV), zinc oxide (ZnO) is a promising candidate for the development of light-emitting devices, laser diodes, gas detectors. ZnO films are widely used as anti-refrective and window layers of solar cells based on absorbing layers of Si, CdTe, CIGS and CZTSe.

Due to the possibility of obtaining condensates with controlled structural characteristics (nanodots, nanorods, etc) among the various techniques of zinc oxide films obtaining, chemical bath deposition (CBD) is very promising method [1]. For practical use of ZnO, it is necessary to obtain films with optimized structural and substructural characteristics, and controlled elemental composition. That is why the purpose of the research, is to study elemental, phase composition; structure and substructure of ZnO condensates, obtained by CBD from an aqueous solution, depending on the physical and chemical conditions of the deposition.

Experimental details

Investigation of phase composition, structural and substructural properties of ZnO films, obtained by CBD with different duration from zinc nitrate and ammonia, are presented in the work. Deposition of thin films was carried out onto pre-cleaned glass. Temperature of solution was 90 ºC. The duration of the deposition varied in the range from 30 to 120 minutes. Detailed procedure of the films synthesis is described in the [1]. Effect of deposition time on the structure and substructure of condensates was studied using scanning electron microscopy, XRD analysis and Raman spectroscopy.

Interpretation of experimental results

It is shown that after the deposition for 60 min it is formed a densely packed array of ZnO nanorods. Synthesized ZnO nanorods have form as a hexagonal prisms with diameters (0.2 - 0.8 μm), length (2.0-3.5 μm), and different angle to the substrate. It is established that increasing of deposition time to 90 min (Fig.1 a) leads to increase thickness (1.0 - 1.9 μm) and length (4.8-6.7 μm) of nanorods. Increasing of the deposition time to 120 min (Fig.1 b) leads to formation of a continuous film.

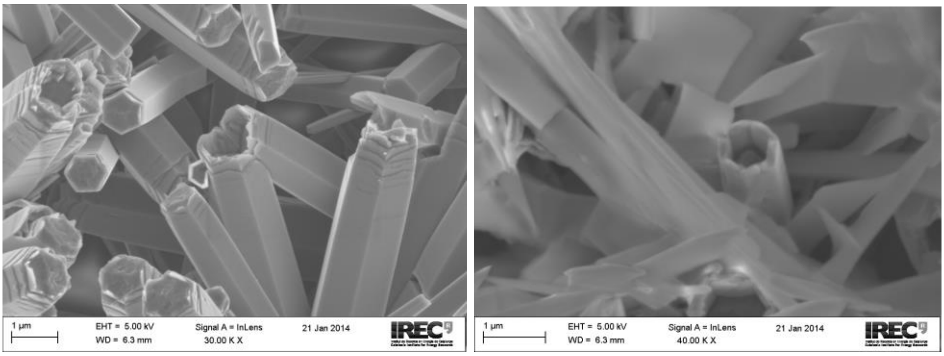

Fig. 1. SEM images of films of ZnO deposited with duration τ of 90 min (a) and 120 min (b).

Pole density and orientation factor calculations shown that condensates have a hexagonal structure with (*f* = 2.31-6.01) growth texture of [002]. The values of the lattice constants depend on the time of deposition and film thickness, respectively. With increasing condensation time, lattice constants increased from *a* = 0.32486 nm, c = 0.52087 nm to *a* = 0.32538 nm, c = 0.52149 nm. Calculation of the unit cell volume (*V*) showed that increasing the deposition time leads to an increase of $V = (47.60 \cdot 10^{30} - 47.81 \cdot 10^{30})\ m^{-3}$. Coherent scattering domain size (CSD) and level of microstrain in ZnO films in the direction perpendicular to the crystallographic planes (002) were *L* ~ 26-42 nm and $\varepsilon \sim (0.59\text{-}3.09) \cdot 10^{-3}$ respectively, and decreased with increasing of deposition time of thin layers.

In the Raman spectra of samples there were detected an intense peaks at frequencies of 339, 439 and 578 cm^{-1}, which were interpreted as 2E2 (low), E2 (high), A1 (LO) phonon modes of ZnO.

Conclusion

It was established that a growth of ZnO condensates occurred through the formation of nanorods with hexagonal structure, texture growth of [002] and lattice constants of *a* = 0.32538 nm, *c* = 0.52149 nm. Value of CSD and level of microstrrain were, respectively, *L* ~ 26-42 nm and $\varepsilon \sim (0.59\text{-}3.09) \cdot 10^{-3}$ and determined by deposition regimes. As a result, we selected the regimes of condensates deposition with single-phase structure. In addition, it was found that by changing the deposition time we can synthesize ZnO layers with pre-defined structural properties from nanorods to continuous films for creation of optoelectronic devices.

References

[1] A. S. Opanasyuk, T. O. Berestok, P. M. Fochuk, A. E. Bolotnikov, R. B. James, Proc. of SPIE 8823 (2013) 88230Q-1.

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