AFM topography of ZnO_X:MgO nanocomposite sol-gel films on the surface of silicon

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Abstract
The results of determining by AFM the parameters of sol-gel synthesis influence for the formation of nanocomposite coatings ZnO_x:MgO with a band gap greater than 5 eV and with high sensitivity to UV and visible radiation are presented. It is shown that depending on the magnesium concentration, change in the surface of the ZnOx: Mg films is observed.

Introduction

The search for new materials for such sensors with sensitivity to UV radiation is an urgent task. Among the requirements imposed on such materials, along with high thermal stability, radiation and chemical resistance, the value of the band gap is important. It should be noted that the structural parameters of oxide layers of complex composition are determined mainly by the conditions and modes of their formation. An analysis of the technological methods used in the synthesis of wide-gap semiconductor materials [1, 2] indicates a number of advantages when using the sol-gel method for these purposes.

When choosing an alloying addition, the radius of the alloying element must be approximately equal to the radius of the element to be replaced and, as a result, a compound with slight distortions of the crystal lattice is formed. The radius of the Mg^{2+} ion (0.57 A) is comparable to the radius of the Zn^{2+} ion (0.60 A), which makes magnesium suitable as a dopant to replace Zn in its lattice and facilitate the increase in the band gap [2].

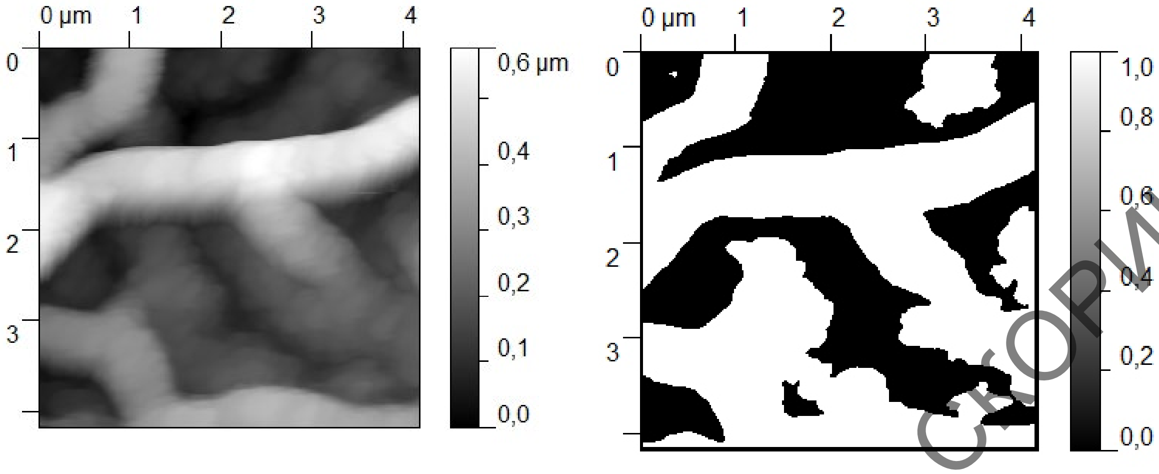
Experimental

Layers based on ZnO:Mg films were obtained by sol-gel method using separate hydrolysis. The application method was centrifugation. The starting materials used were zinc acetate dihydrate (ZnAc) [Zn $(CH_3COO)_2 \times 2H_2O$]; magnesium acetate (Mg $(CH_3COO)_2$); isopropyl alcohol; distilled water [H_2O]; diethanolamine (DEA) [$HOCH_2CH_2NHCH_2CH_2OH$]. The film-forming solution (POR) was prepared as follows: zinc acetate and magnesium acetate were separately dissolved in isopropyl alcohol and stirred at 60 ° C for 10 minutes. When the solution was transformed into an emulsion, diethanolamine was added at a molar ratio DEA / ZnAc 1: 1 and H_2O / ZnAc 2:1, respectively. A sol based on magnesium acetate was prepared in a similar way. Then the sols were mixed in different concentrations to obtain films with different component ratios (1:1, 1:2, 1:5). Three variants of the sol were prepared: hydrochloric acid was additionally added to sol № 1 and nitric acid to sol №. 3. The deposition of the film was carried out by centrifugation at a rotation speed of 2000 rpm for 40 s, followed by drying each layer at 60 °C for 10 minutes (2 layers). The final heat treatment was carried out at temperatures of 250 °C and 450 °C for 30 minutes. Sols containing acetic acid (series 2) did not provide adhesion to the substrate surface.

Results and discussion

Fig. 1 shows typical AFM images of the surface topography of ZnO_x:MgO films on the surface of monocrystalline silicon. The surface of the obtained oxide film №3(1:1) is characterized by developed relief with a high degree of roughness and packing of crystallites according to the “moiré” structure. The topography of the surface of this sample indicates the formation of two separate phases, as evidenced by the data in Table 1. Film №1(1:1) without visible pores and punctures is formed by pyramidal crystallites with the same growth direction perpendicular to the plate. The synthesized films had high adhesion to monocrystalline silicon surfaces. The average grain size on the surface of ZnO_x:MgO films is about 200 μm, and the roughness is

0.114 µm. For films №. 3 (1:1) ZnO, the size and shape of the grains increases 6 times, the roughness – 1.5 – 2 times.



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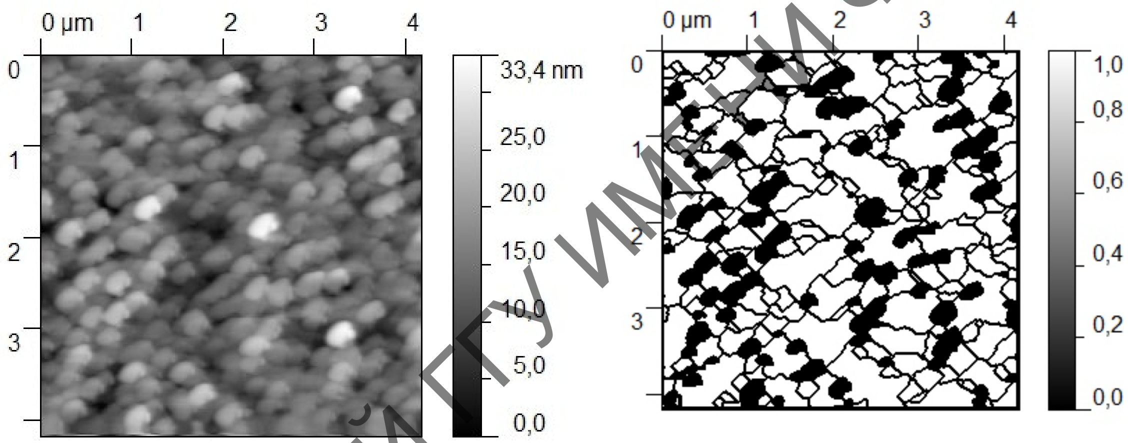

№1(1:1)

Fig. 1. AFM images of the surface topography of ZnO_x:MgO films

Table 1. Parameters of the surface and band gap of ZnO_x:MgO films

ZnO:Mg sample №	№1 (1:1)	№3 (1:1)
Ra, nm	3.5	114
Average grains size, nm	174	1060
Band gap, Eg, eV	3.31	3.28/4.72

Conclusion

Samples of coatings based on ZnO_x:MgO were studied using AFM. The Gwyddion program calculated the surface roughness, the number of grains and their average size. It was found that the average grain size on the surface of ZnO films is about 200 µm, and the roughness is 0.114 µm. For films №. 3(1:1) ZnO_x:MgO, the size and shape of grains increases 6 times, roughness – 1.5 – 2 times compared to sample № 1(1:1). The use of nitric acid leads to appearance of two separate oxide phases and to change of the size and shape of the particles ZnO_x:MgO.

References

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[2] K. Gu [et al.] "Tailoring microstructure and optical properties of MgZnO film on glass by substrate temperature", Materials Letters. P– 128416. 2020.