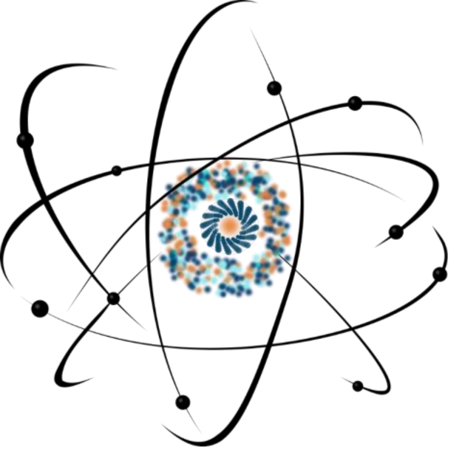

ELECTRONIC STRUCTURE OF ZINC OXIDE THIN FILMS DOPED WITH NITROGEN AND FLUORINE

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Idea

Use of the X-ray photoelectron spectroscopy(XPS) method to investigate the electronic structure of zinc oxide thin films before and after fluorine and nitrogen doping.

Method

X-ray spectrometer:"JEOL" JSPM-4610. Work pressure no less then 10^{-7} Pa.
X-ray source Al K_{α} 1486.3 eV. Energy resolution 0.1 eV.

Introduction

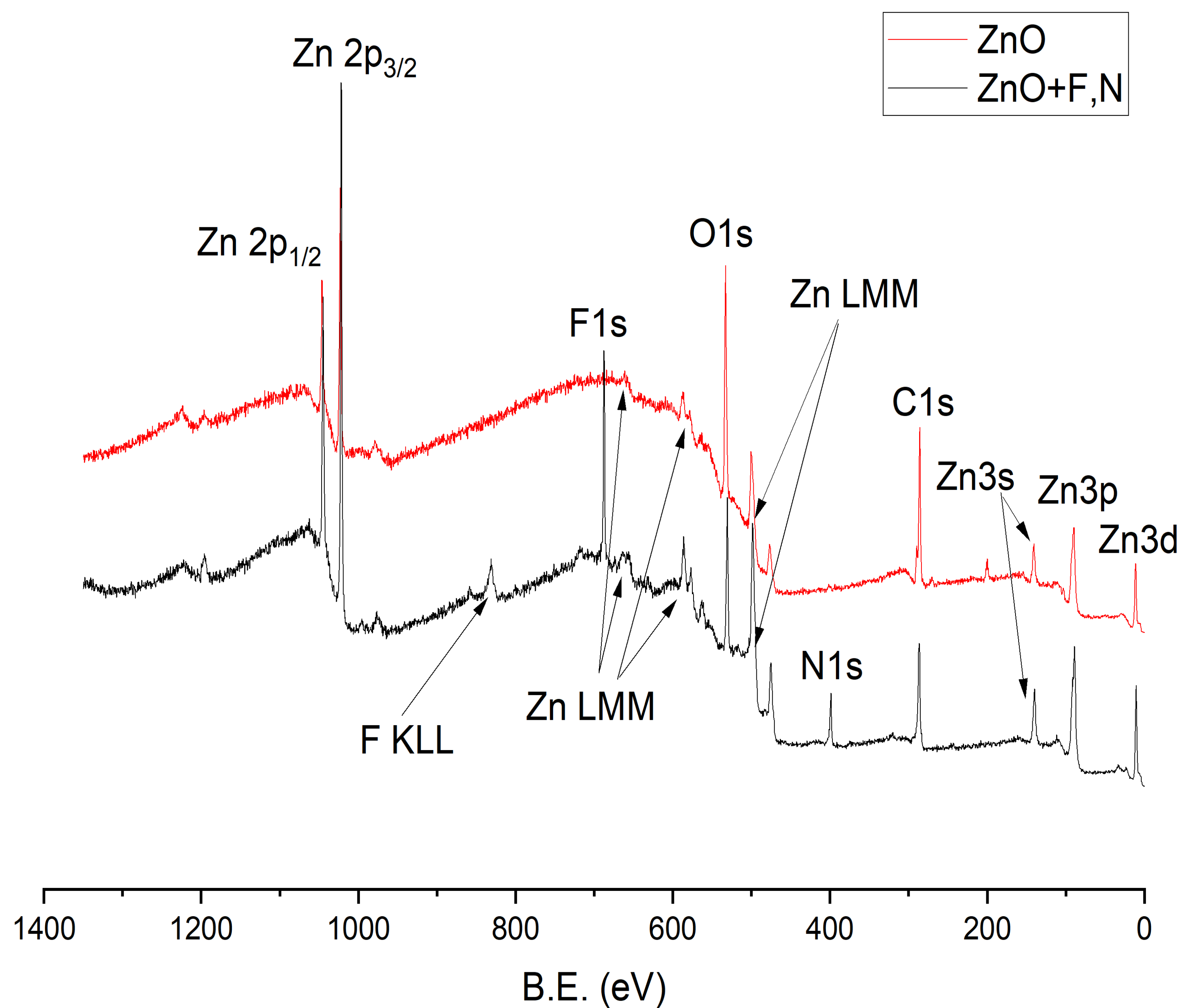
ZnO films are attracting attention due to their unique optical and electrical properties as well as their wide range of applications. A wide bandgap of up to 3.37 eV and a transparency of about 80% in the visible range and low electrical resistance make them a potential candidate for use in solar cells as a transparent conductive electrode. However, today, the transparency and electrical conductivity of ZnO films are still lower than that of the widely used and expensive tin doped indium oxide (ITO). After fluorine doping of zinc oxide thin films, an increase in transparency and a decrease in resistivity were observed [1]. therefore, optimization of the processes of obtaining ZnO films by doping with various elements, in particular, fluorine and nitrogen, in order to improve physical properties is an essential task.

Sample preparation

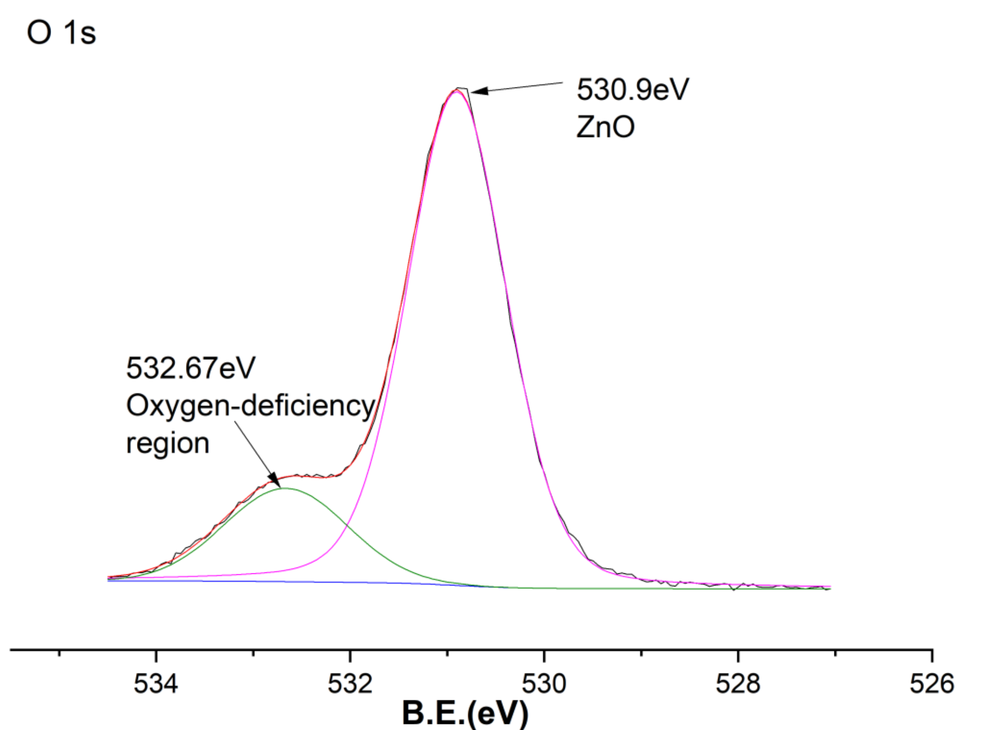
In this work, ZnO films were prepared by magnetron deposition from ZnO target and doped with fluorine by placing fluoroplastic in a chamber. Nitrogen was present in the plasma atmosphere by injection from the gas phase.

Result

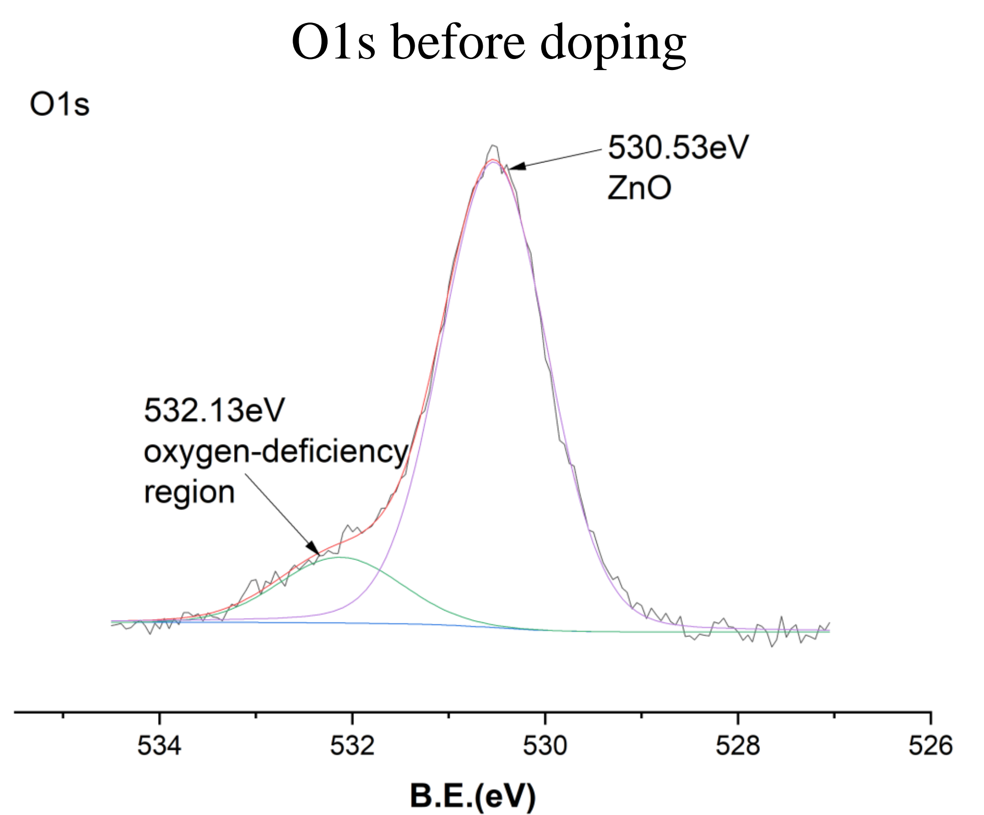
XPS revealed the presence of only Zn, O, C, and N and F in the doped samples, indicating a successful doping procedure. The value of the modified Auger parameter for Zn L3M45M45 was 2010.1-2010.3 eV, which, when compared with the corresponding parameters of the NIST database [2], indicates the presence of only Zn-O bonds. Thus, zinc does not interact with fluorine and nitrogen. The XPS spectrum of oxygen was decomposed into two components, the peak with a lower binding energy characterizes ZnO, the peak with a higher binding energy corresponds to oxygen with broken bonds. After doping with nitrogen and fluorine, a decrease in the intensity of the high-energy oxygen peak was observed, which may indicate a decrease in the number of oxygen vacancies. Given that nitrogen and oxygen have almost the same atomic radius, and fluorine has an even smaller atomic radius, it can be assumed that nitrogen and fluorine atoms diffuse into the oxygen-deficient regions, thereby reducing the number of defects in the film.



Wide spectra of ZnO thin film before doping (red line) and after doping with nitrogen and fluorine (black line)



O1s before doping



O1s after doping

Conclusions

The successful doping of the films with nitrogen and fluorine was established by the XPS method. After doping, a redistribution of the intensity in the O 1s spectrum of oxygen and a decrease in the O 1s binding energy are observed. Also, the decrease in the intensity of the high-energy oxygen peak after doping may indicate a decrease in the number of oxygen vacancies. Considering that nitrogen and oxygen have almost the same atomic radius, and fluorine has an even smaller atomic radius, it can be assumed that nitrogen and fluorine atoms diffuse into oxygen-deficient regions, thereby reducing the number of defects in the film.

[1]Han Yanbing; et. al. *Influences of nitrogen doping on the electrical characteristics of Indium-Zinc-Oxide thin film transistors. // IEEE Transactions on Device and Materials Reliability. - 2016. - 16. I 4.-P. 642-646.*

[2]NIST X-ray Photoelectron Spectroscopy Database, NIST Standard Reference Database Number 20, National Institute of Standards and Technology, Gaithersburg MD, 20899 (2000).