SPECTRAL AND X-RAY STUDIES OF INDIUM OXIDE FILMS ON SAPPHIRE SUBSTRATES

A.A. TIKHII[1]*, YU.M. NIKOLAENKO*[2]*, YU.I. ZHIKHAREVA*[3]*, I.V. ZHIKHAREV*[2]

[1] *Lugansk Taras Shevchenko National University, Oboronnaya str., 2, Lugansk 91011, Ukraine*
[2] *Donetsk Institute for Physics and Engineering named after A.A. Galkin, Rozy Lyuksemburg str., 72, Donetsk, 83114 Ukraine*
[3] *Taras Shevchenko National University of Kyiv, Volodymyrska str., 64/13, Kyiv, 01601, Ukraine*

Optical transmission spectra and X-ray diffraction of thin In_2O_3 films deposited by dc-magnetron sputtering on Al_2O_3 (012) substrates are investigated.

The diffraction patterns exhibit the presents of the (222) reflex of cubic In_2O_3 (space group Ia-3). Its position shifts from 30.3 to 30.6°, with a decrease in the film thickness. The half-width of this reflex decreases with decrease of the deposition time, which may indicate an increase in the crystallite size of the film material.

The results of optical transmittance measurements demonstrate its anomalous decrease with decreasing wavelength. Moreover, an interference pattern is observed on the optical transmission curves of thick films, even in the low transmission region. The three layers model of the investigated films was proposed to explain these results. The optical properties of the middle layer correspond to the cubic modification of In_2O_3 according to [1]. The film surface was assumed to be rough, and modeled as a homogeneous layer with optical properties calculated based on the dielectric constant of a cubic modification of In_2O_3 and a fill factor of 0.5. The best fit of the spectral dependence of extinction coefficient of third layer is the law of the fundamental absorption in a semiconductor with band gap of 1.39 eV for direct transitions. The refractive index of this layer was assigned the same spectral dependence of the refractive index as for the film material.

The thicknesses of all layers were choosing manually to agree the calculated transmission spectra with the measured spectra of the films. The calculations are performed using the scattering matrix for a system of plane-parallel homogeneous isotropic layers [2]. A comparison of the optical transmittance calculated within the frame of the proposed model with the measurements shows good agreement.

The total thicknesses of the films were found to be from 97 to 392 nm (deposition time: 15 – 180 min). The thickness of the rough layer on the film surface (~ 60 nm) is practically independent of the deposition time and is mainly determined by the deposition mode. The thickness of the film-substrate transition layer (~ 35 nm) practically does not depend on the deposition time also, and, therefore, its appearance is completely due to the influence of the surface of the substrate. The formation of this layer, presumably, does not require a large violation of the stoichiometry of the film, since it is possibly related to the blurring of the band gap due to the large number of defects in the crystal structure, as well as the formation of impurity levels inside the band gap.

REFERENCES

[1] A. Schleife, M.D. Neumann, N. Esser, Z. Galazka, A. Gottwald, J. Nixdorf, R. Goldhahn, M. Feneberg, Optical properties of In_2O_3 from experiment and first-principles theory: influence of lattice screening, New J. Phys. vol. 20, Article Number 053016, 2018. http://dx.doi.org/10.1088/1367-2630/aabeb0.

[2] H.G. Tompkins, E.A. Irene (Eds), Handbook Of Ellipsometry, William Andrew Publishing, USA, 2005.