Magnetron sputtered YHO thin film oxydation dynamics and optical properties

M. Zubkins, I. Aulika, E. Strods, V. Vibornijs, L. Bikse, J. Purans
Institute of Solid State Physics, University of Latvia, Kengaraga 8, LV-1063, Riga, Latvia

Yttrium and other rare-earth (RE) metal oxy-hydrides (YHO, REHO – notations referred in the text hereinafter, in principle, is irrespective to the stoichiometry) are a new class of inorganic mixed-anion materials [1], which exhibit a photochromic effect and a light-induced resistivity change at room temperature and ambient pressure. These switchable optical and electrical properties enable their utilization in a multitude of technological applications, such as energy-saving smart windows, sensors, ophthalmic lenses, and medical devices. Recently reported studies show that the modification of the deposition parameters causes significant changes in the composition of REHO films, accompanied by a varying optical properties.

In order to tune and fully exploit REHOs in applications, further progress requires: reaction conditions for film synthesis have to be investigated carefully, including the film oxidation kinetics and the characterization of the oxy-hydride phase.

In this work, the films were fabricated on soda-lime glass using the vacuum PVD coater G500M (Sidrabe Vacuum, Ltd.) at various sputtering pressure (SP) from 3 mTorr up to 20 mTorr. Detailed characterisations by profilometer CART Veeco Dektak 150, X-ray diffractometer with Cu Kα radiation, Rigaku MiniFlex 600, high-resolution dual-beam scanning electron microscope Thermo Scientific Helios 5 UX, and spectroscopic ellipsometer WOOLLAM RC2 were performed.

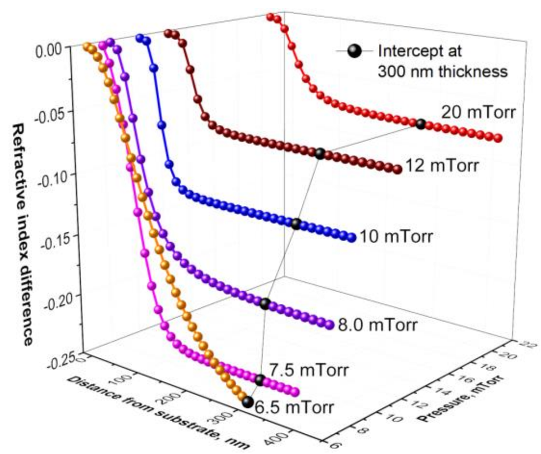

Fig. 1. Optical depth profile (at 1.669 eV or 742.8 nm) of thin films sputtered at different pressures.

For the first time in-situ oxidation dynamics were observed by means of the transmittance measurements just after the deposition of the films by introducing the oxygen in the sputtering chamber. Transmittance increases and oxidation time constant rapidly decreases with increase of the film SP. XRD analysis show that the crystallographic structure of the film is just slightly affected by the SP: with increase of the SP the intensity of the peak around 29° of 2θ is decreasing thus films undergo compositional changes rather than structural. The SP ~(6.0-6.5) mTorr was found to be a critical pressure, where the refractive index *n* extinction coefficient *k* dispersion curves completely change the characteristic from metallic to semiconductor/dielectric behavior with Tauc optical band E_g around (2.5-2.8) eV. Moreover, all films fabricated at SP higher than this critical pressure exhibit optical gradient (Fig.1): *n* decreases in direction from the bottom to the top of the films, and the lower is the SP, the higher is the *n* difference within the depth of the films. For all films, the E_g and *n* increases and *k* decreases with increase of SP.

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[1] Kageyama, Hiroshi, et al., Nature communications 9.1 (2018): 1-15.