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RF sputtering of oxide films in Ar and Ar-H2 gas mixtures: role of H incorporation in developing transparent conductive coatings.

Gloria Gottardi[1], Ruben Bartali[2], Victor Micheli[2], Ioana Luciu[3], Nadhira Laidani[2]

[1]Fondazione Bruno Kessler, Povo (Trento), Italy [2]Fondazione Bruno Kessler, Povo (Trento), Italy [3]Fondazione Bruno Kessler & Università di Trento, Povo (Trento), Italy

ggottard@fbk.eu

Fundamental and applied investigation of ZnO and TiO_2 has been recently experiencing a renaissance due to the prospective use of such materials in various technological domains and, in particular, as transparent conductive oxides (TCOs) for solar cells applications. In this respect, the present work aims to study the structural and physical properties of ZnO and TiO_2 thin films deposited by RF sputtering. Different gas mixtures were explored. Specifically, pure Ar and Ar-H_2 at various concentrations were used to grow the films on n-type Si (100) wafers and glass without external heating.
The plasma chemical species were followed in function of the different gas mixture settings by optical emission spectroscopy (OES). X-ray photoelectron spectroscopy (XPS) and ATR-FTIR (Attenuated Total Reflection Fourier-Transformed Infrared) spectroscopy were used to study the bulk and surface chemical composition of the films, while X-ray Diffraction (XRD) analysis allowed lattice structure and grain size determination. The films were also characterized for their electrical and optical properties.
The introduction of hydrogen in the plasma phase strongly affected the structural and physical properties of the films. In the case of ZnO films, in particular, both FTIR spectra and X-ray diffraction patterns showed that all the films crystallized in the hexagonal würtzite form. Nevertheless, while samples deposited in pure Ar plasma presented just one dominant preferred orientation along the [002] axis, films sputtered in Ar:H_2 atmosphere exhibited multiple growth directions with crystallites of noticeably reduced dimensions. Such a structural modification turns up together with a pronounced change in the films electrical behaviour, which become conductive when H is added in the gas mixture. By combining XPS, ATR-FTIR and OES data we could correlate the established conductivity and its variations with ZnO doping by intentional H incorporation in the crystal structure. Hydrogen in ZnO structure was found in the form of hydroxide chemical state.
Comparative studies were performed with respect to TiO_2 films.

Keywords
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