PO2075

Coordination chemistry of titanium and zinc in Ti(1-x)Zn2xO2 (0≤x≤1) ultrathin films grown by DC reactive magnetron sputtering

Miriam Yuste[1], Ignacio Caretti[1], Ricardo Torres[1], Olga Sánchez[1], Ignacio Jiménez[1], Ramón Escobar Galindo[1]

[1]ICMM-CSIC, Cantoblanco, Madrid, Spain

miriam.yuste@icmm.csic.es

Transition metal doping and formation of mixed oxides are widely used mechanisms to improve the intrinsic properties of binary oxides. Both procedures have been decisive to explain the spectacular increase of applications based on ZnO and TiO_2 films (optoelectronics, photovoltaic and dye sensitized solar cells, gas sensors, high frequency dielectric materials, etc.). The vast majority of previous work on doped ZnO films is related to doping with group III elements (Al, Ga, In) but fewer studies have been performed on quadrivalent dopants as titanium, which have one more valence than the trivalent cations and can provide two free electrons per atom to improve the conductivity of the ZnO host. In turn, the mechanisms driving the formation of the different zinc titanate compounds in the ZnO–TiO_2 system are still under debate. Ultrathin films (thickness < 40nm) with $Ti_{(1-x)}Zn_{2x}O_2$ (0+ ions to make use of the cross section resonance ^{16}O (α, α) ^{16}O at that particular energy. X-ray Absorption Near Edge Structure (XANES) analysis of the (Ti, Zn) L-edges and O K-edge revealed clear changes in the bonding structure of ZnO films for increasing Ti load. In this way, the coordination chemistry of Ti^{4+} and Zn^{2+} cations was examined for a wide range of oxide compositions. We observed a transition from octahedrally coordinated Zn^{2+} in a mixed oxide *h*-$ZnTiO_3$ like structure to the expected tetrahedral symmetry of this cation in Ti-doped ZnO (TZO) films with a wurtzite (*w*) phase. Regarding Ti^{4+}, a similar change from octahedral to tetrahedral sites is detected in the transition from *h*-$ZnTiO_3$ to TZO coatings. Therefore, Ti is incorporated as dopant by substituting Zn atoms in the *w*-ZnO structure. The optimum Ti doping was found to be 0.5 at.%, for which the TZO sample showed a much lower resistivity than the more insulating ZnO films.

Keywords
XANES
RBS
ZnO
TiO2
coordination chemistry