Effects of in-situ post-annealing process on microstructure, electrical properties, and chemical bonds of Li-doped ZnO thin films deposited by RF magnetron sputtering system

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Zinc oxide (ZnO) is a direct wide-bandgap (E_g~3.37 eV) multifunctional semiconductor material with unique electrical, optical, acoustic, and mechanical properties and a large exciton binding energy (~60 meV). It has a hexagonal wurtzite crystal structure, which makes it piezoelectric. Since the early 1970s, it has been used for thin film piezoelectric devices due to its ease of deposition and large surface area [1]. Recent works on ZnO thin films have observed better piezoelectricity and ferroelectricity after doping with certain metals , e.g., Fe, Co, Cu, Ni, and Li [2-4]. Among these dopants, Li is used in the present study due to the ionic radii disparity between the host Zn^{2+} ions (0.74 Å) and the dopant Li^{+} ions (0.6 Å). Depending on this ion size disparity, Li atoms can occupy off-center positions to enhance the permanent electric dipoles.

In this article, 3 at% Li-doped zinc oxide (LZO) thin films are deposited onto Pt/Ti/SiO_2/Si substrates via radio frequency (RF) magnetron sputtering method. The structure evolution with annealing temperature of the predominantly (002)-oriented LZO films after in-situ post-annealing process is determined. The largest value of the piezoelectric coefficient (d_{33}) (22.85 pm/V) are obtained for LZO films post-annealed at 600°C, which can be attributed to the predominant (002)-oriented crystalline structure, the release of intrinsic residual compressive stress, and less non-lattice oxygen. Moreover, this article is suggested as a poster.

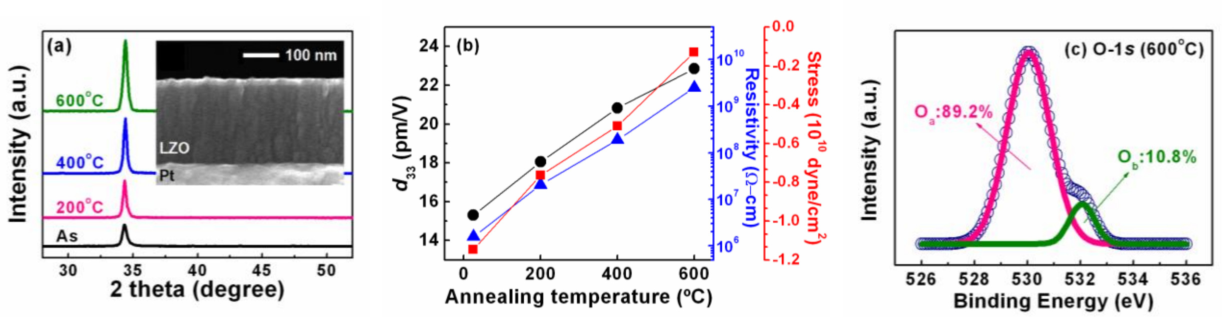

Fig. 1 (a) X-ray diffraction patterns of LZO thin films post-annealed for various temperatures. The inset shows the cross-sectional SEM image of the sample annealed at 600°C, (b) effective piezoelectric coefficient d_{33} response, resistivity, and intrinsic stress calculated from the XRD patterns, and (c) XPS spectrum of O-1*s* core level of the sample annealed at 600°C LZO films (O_a is attributed to O^{2-} ions in the stoichiometric wurtzite ZnO structure whereas O_b is attributed to non-lattice oxygen) [5].

In summary, a large piezoelectric coefficient d_{33} value of 22.85 pm/V was obtained for 3 at% Li-doped ZnO films deposited using RF magnetron sputtering and in-situ post-annealed at 600°C. The improvement in the piezoelectric properties can be ascribed to the predominant (002)-oriented crystalline structure, the release of intrinsic residual compressive stress and less non-lattice oxygen. LZO thin films are thus a promising candidate material for high-density piezoelectric devices.

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