3D nanoscale spatial imaging of doped ZnO and TiO_2 transparent thermoelectric thin films

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Transparent thermoelectric materials are a promising technology for touchscreen displays and solar cell applications, rendering a sustainable powering of the device. In order to enhance the thermoelectric performance, the material must have a high Seebeck coefficient and high electrical but low thermal conductivity. This work focuses on the effect of doping on ZnO and TiO_2-based thin films deposited by DC magnetron sputtering. The properties of the films depend strongly on the dopant type and concentration. On the one hand, it has been documented that Al and Ga doping can improve the electrical properties in ZnO, as can Nb doping in TiO_2. On the other hand, introducing heavier elements (such as Bi, Sb or Nb) into the metal-oxide matrix hinders phonon mediated heat conduction, and consequently reduces the thermal conductivity, which is a promising approach. Atom Probe Tomography and Time-of-Flight Secondary Ion Mass Spectrometry are powerful tools to determine the composition and inherent homogeneity within the thin films, as well as to investigate the cation and anion segregations to interfaces and grain boundaries. For the ZnO-based films, Al and Ga dopants are homogeneously distributed within the crystals, with the exception of Bi, which is not incorporated in the ZnO wurtzite cell and segregates at the grain boundaries and at the triple junctions (Figure 1 a). Thus, Bi contributes to grain boundary scattering of phonons and contributes less to the reduction of the thermal conductivity, in comparison to Ga-, Al-, and Sb-doping in ZnO. For the Sb-doped ZnO thin films, a larger Zn content was registered at the triple junctions of the grain boundary. As for the Nb-doped TiO_2 thin films, Nb is homogeneously distributed into the TiO_2 matrix and no grain boundaries are visible. However, the composition varies depending on the deposition conditions, where the Nb content inside the film changes depending on the oxygen content controlled through the reactive O_2 flow during the sputtering depositions (Figure 1b).

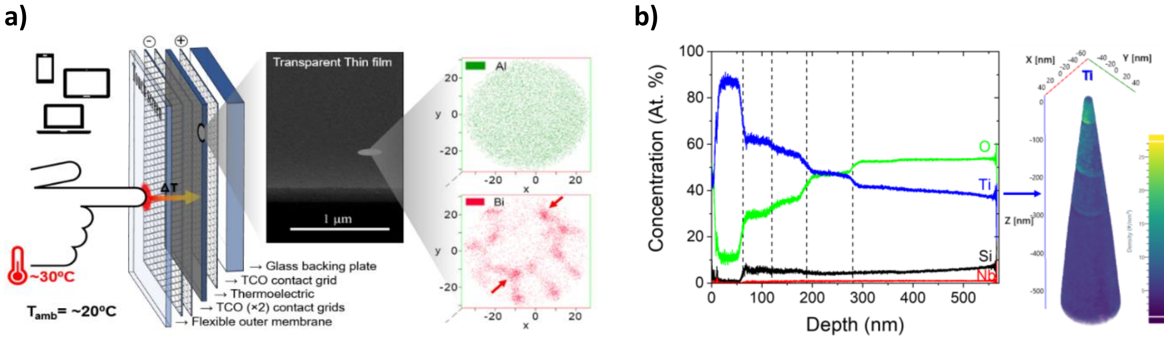

Figure 1. **a)** Transparent touch screen prototype featuring a thermoelectric thin film layer. APT reconstruction of ZnO:Al:Bi shows Al homogeneity and Bi segregating to the grain boundaries; b) TiO_2:Nb thin film with varied O_2 flow during reactive sputtering. The Ti content and density increases with an increase of O, while Nb content increases.

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