Electronic Supplementary Information

Influence of hydrogen and oxygen on the structure and properties of sputtered magnesium zirconium oxynitride thin films

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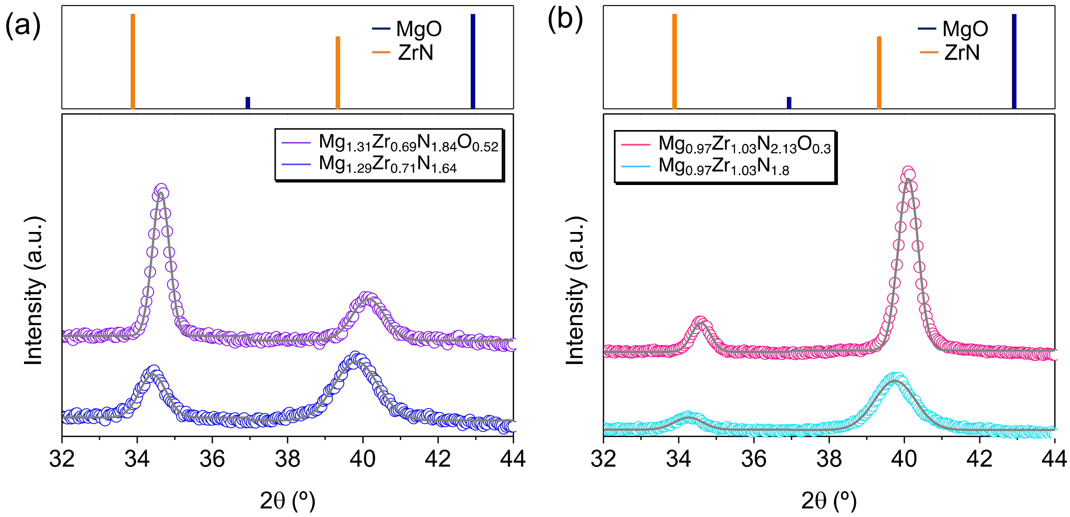

Fig. S1. X-ray diffraction (XRD) pattern for (a) Mg-rich and (b) Zr-rich MZNO thin films for different amounts of oxygen with MgO (JCPDS #45-0946) and ZrN (JCPDS #35-0753) represented above. Circle represents measured XRD, and a solid line represents the Gaussian-fitted curves.

We performed Gaussian fitting to the diffraction patterns in Fig. 2, and they all appeared to be a single peak (symmetric but a bit broad). Furthermore, none of the peaks matches known peaks of MgO (such as (111) at ~36-37° and (200) at ~44-45°.[1],[2]) and ZrN, ((111) was reported to occur at ~33-34° and (200) at ~39-40°.[3]-[5]) In Fig. 2, (111) is at 34-35° and (200) at 40°, which is much more similar to ZrN than MgO. Also, in a line scan from TEM in Fig. S4, it showed relatively homogenous distribution of Mg-Zr-N-O except for grain boundaries in columnar film microstructure, ruling out significant presence of MgO impurities in the bulk of the grains. Overall, the XRD and TEM data suggest that the material should be viewed as ZrN with some dissolved Mg and O. This model is reflected in the MZNO notation we are now using throughout the text.

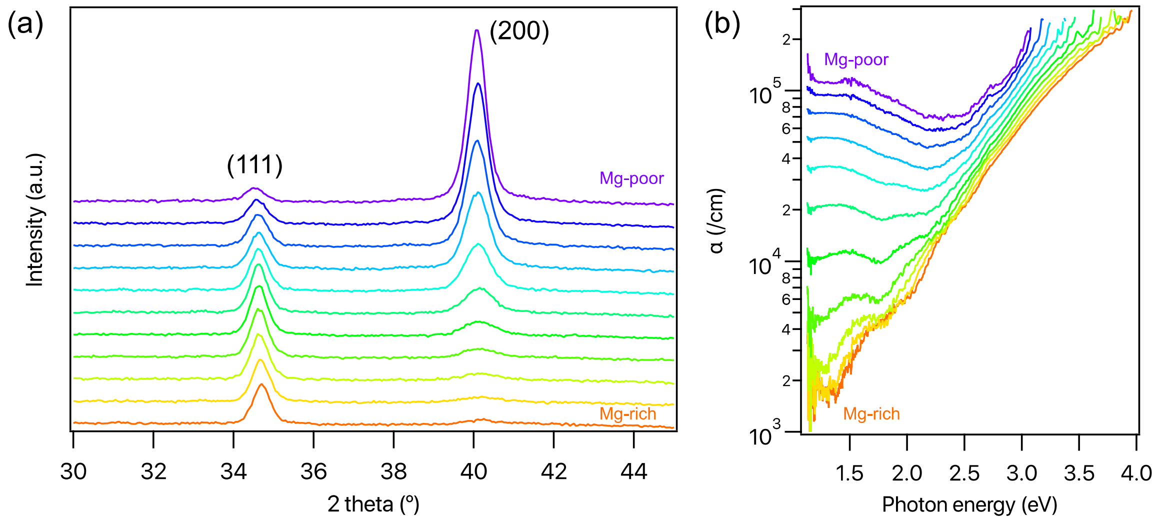

Fig. S2 (a) XRD patterns and (b) UV-vis spectra in MZNO libraries

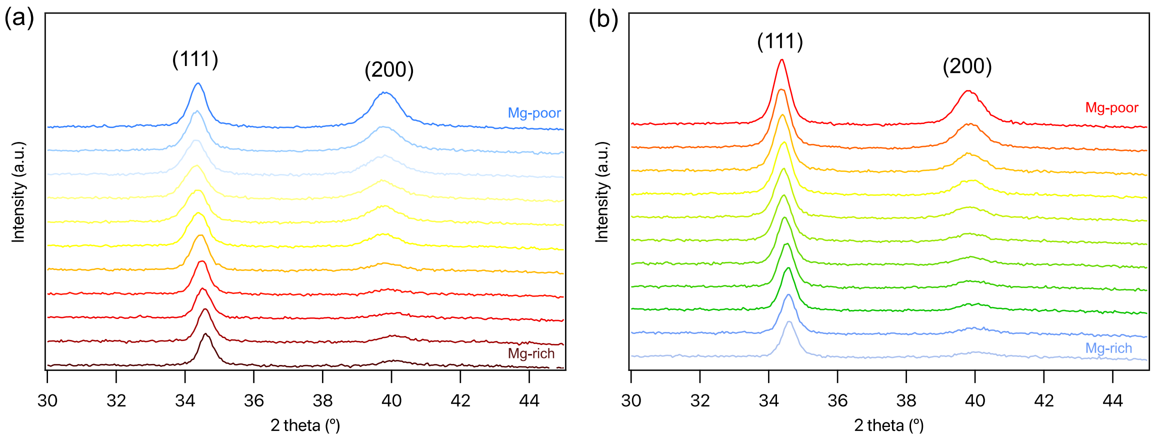

Fig. S3 XRD patterns for MZNO libraries grown (a) without and (b) with hydrogen

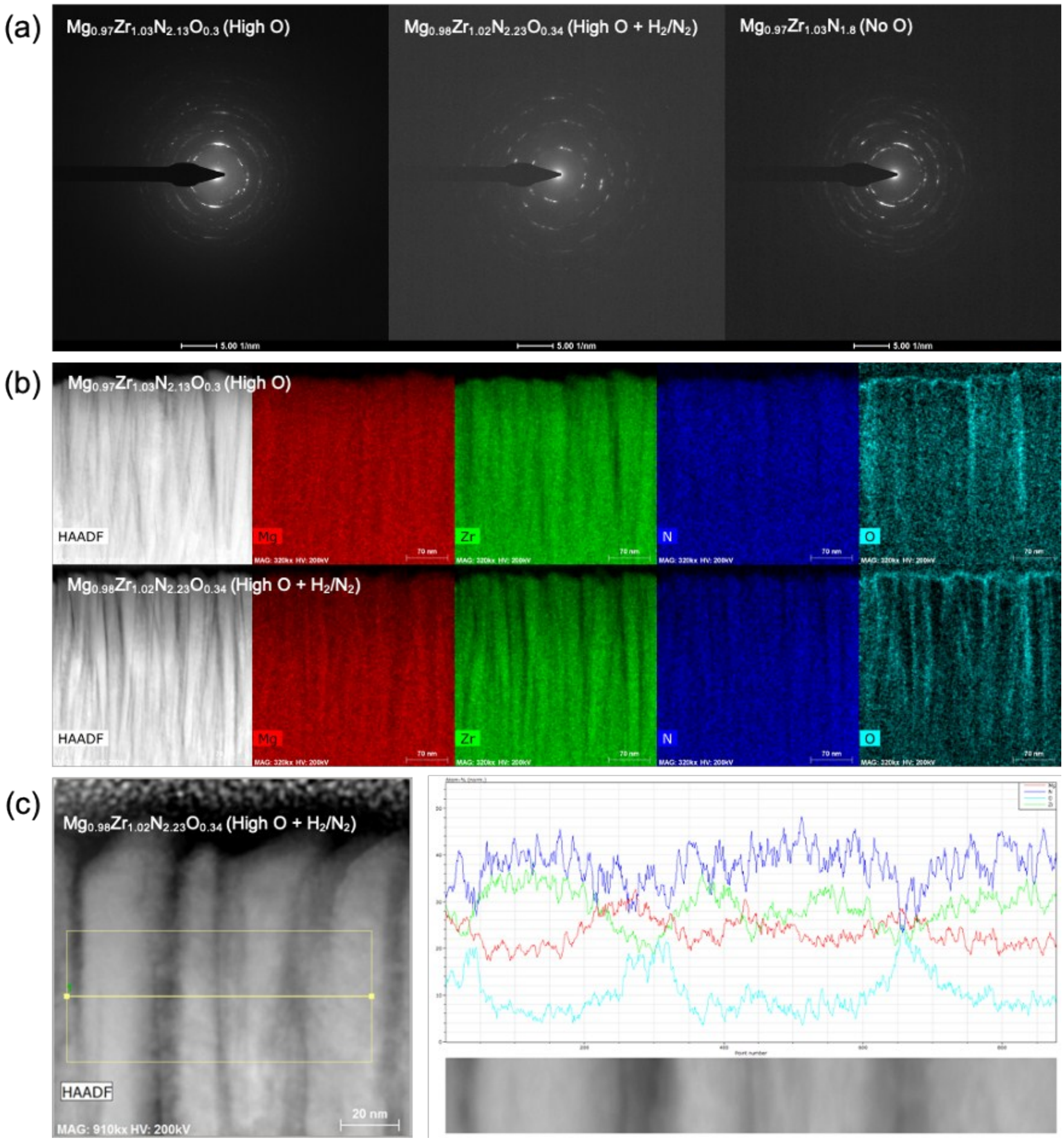

Fig. S4 (a) HAADF images of MZNO thin films before air-annealing, (b) EDS mapping of MZNO thin films after air-annealing, and (c) line-scan for MZNO thin films grown under H_2/N_2. (Mg/(Mg+Zr) = 0.485)

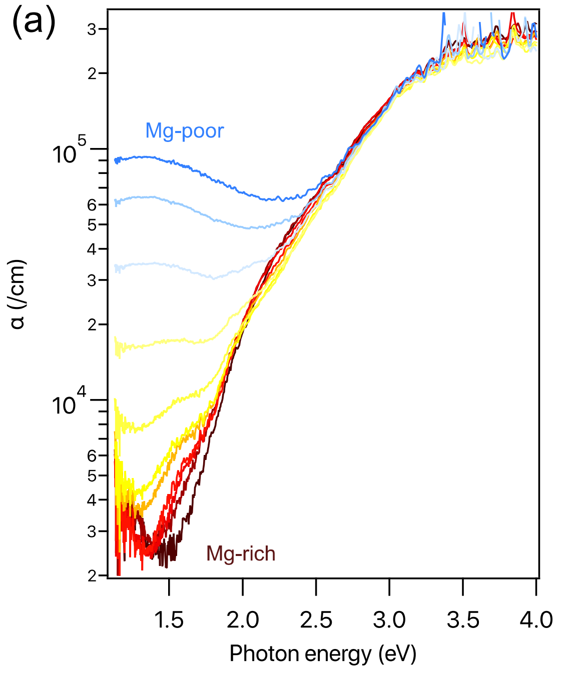

Fig. S5 UV-Vis spectra for MZNO libraries grown (a) without and (b) with hydrogen

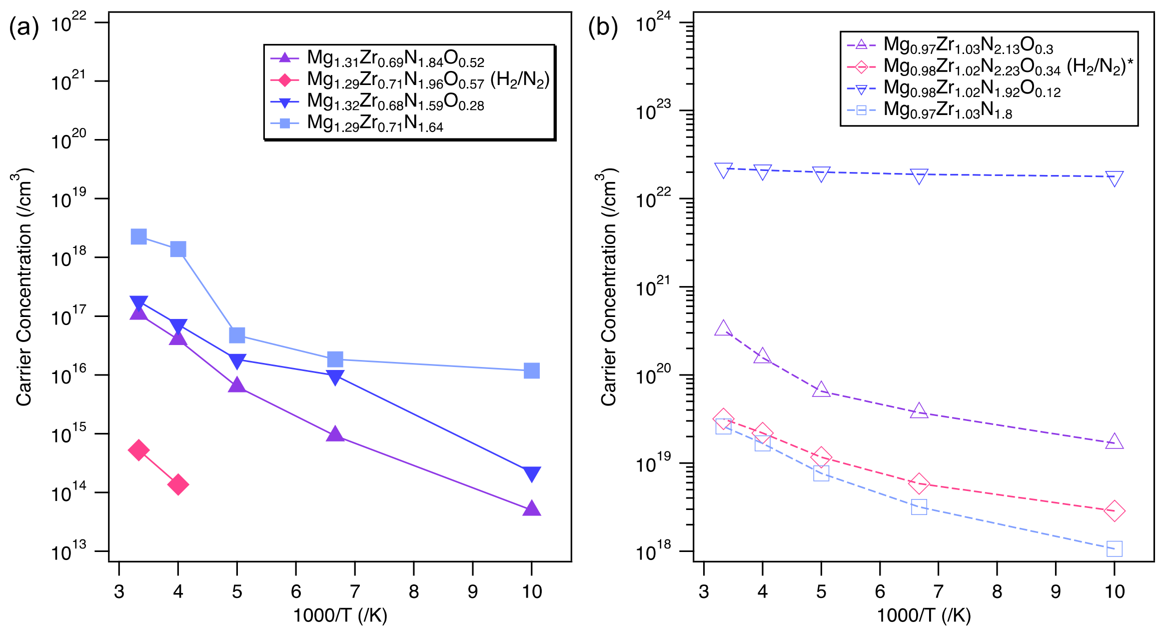

Fig. S6 Change in carrier concentration for (a) Mg-rich and (b) Zr-rich MZNO thin films depending on the amount of oxygen

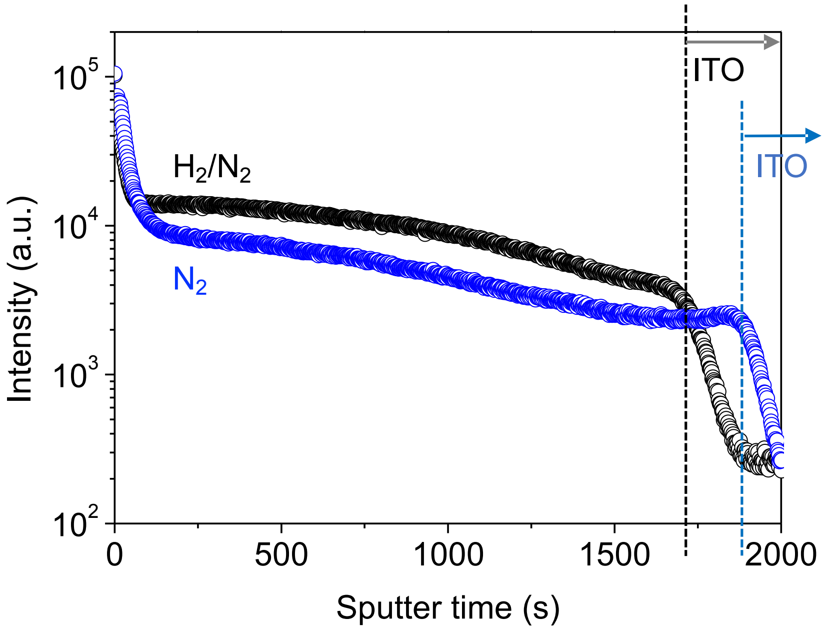

Fig. S7 SIMS depth profile of hydrogen within MZNO thin films on ITO substrate (Mg/(Mg+Zr) = 0.65). The ITO was used as a substrate.

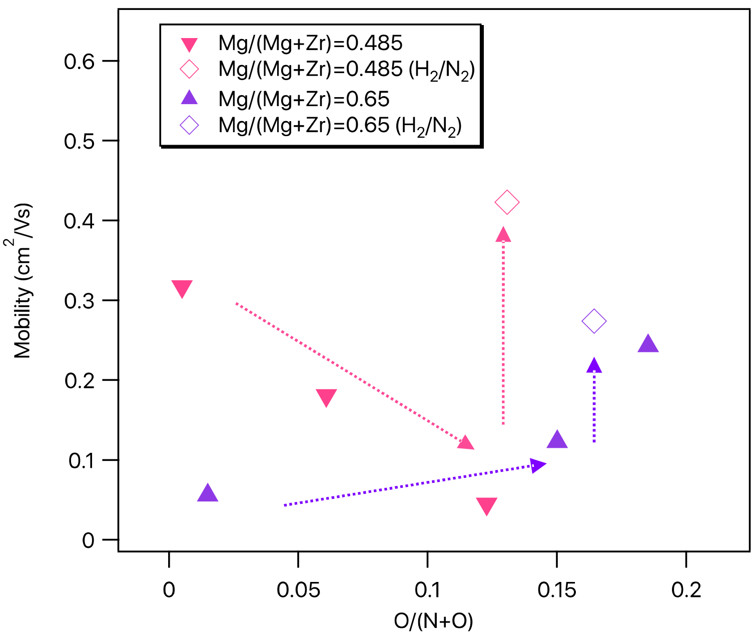

Fig. S8 Change in mobility of MZNO thin films depending on the composition and incorporation of hydrogen

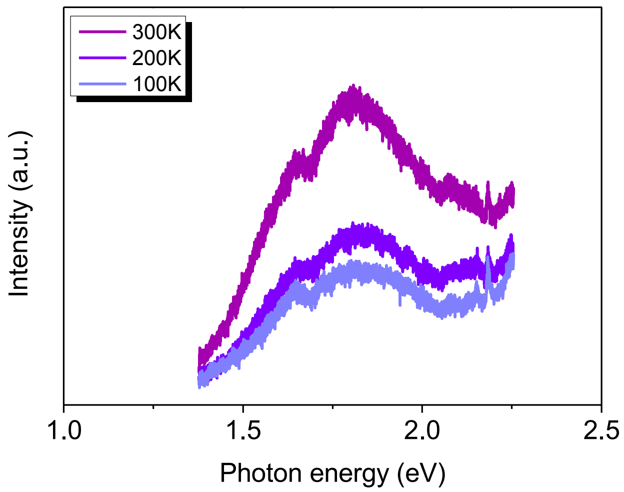

Fig. S9 Temperature-dependent PL spectra for MZNO thin films without hydrogen (Mg/(Mg+Zr) = 0.6)

Reference

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