

# Effect of NH<sub>3</sub> nitridation on the structural, chemical, and optical properties of sputtered Al-doped ZnO thin films

Malihe Ghaffari<sup>1,2</sup>, Omid Sharifamadian<sup>1</sup>, Iryna Matsukevich<sup>1</sup>, Shivangi Chanabhai Dhola<sup>2</sup>, Alexis Duval<sup>2</sup>, Fransizka Scheffler<sup>2</sup>, Orhan Sisman<sup>1</sup>, Dusan Galusek<sup>1,4</sup>, Lothar Wondraczek<sup>2,3</sup>, Jose J. Velazquez<sup>1</sup>

<sup>1</sup> FunGlass Center, TnUAD, 91150 Trencin, Slovakia, [malihe.ghaffari@tnuni.sk](mailto:malihe.ghaffari@tnuni.sk)

<sup>2</sup> Otto Schott Institute of Materials Research, FSU Jena, 07743 Jena, Germany

<sup>3</sup> Center for Energy and Environmental Chemistry, FSU Jena, 07737 Jena, Germany

<sup>4</sup> Joint Glass Center of the IIC SAS, TnUAD, and FChPT STU, 91150 Trencin, Slovakia

Aluminum-doped zinc oxide (AZO) are promising materials for optoelectronic applications regarding their optical transparency, electrical conductivity, and sensitivity to surface interactions. Controlling their defect chemistry and surface properties is important for improving their functional performance. Post-deposition nitridation in an ammonia (NH<sub>3</sub>) atmosphere provides a potential approach to modify these properties through nitrogen incorporation. In this study, AZO films deposited by DC magnetron sputtering under different O<sub>2</sub>/Ar partial pressure, were nitrified at 250 and 450 °C for 3, 8, and 24 h to investigate the influence of deposition conditions and nitridation parameters on their structural, chemical, and optical properties. XRD analysis confirmed that all films preserved the hexagonal wurtzite ZnO structure after nitridation, without detectable secondary phases. The crystallite size, lattice strain, and dislocation density exhibited condition-dependent trends. XPS revealed a single N 1s component centred at approximately 398.5 eV, confirms that nitrogen was successfully incorporated into the near-surface region of the AZO films during NH<sub>3</sub> annealing. NH<sub>3</sub> treatment also enhanced the optical band gap, with values approaching approximately 3.33 eV after nitridation at 450 °C, while Raman spectroscopy revealed nitridation-induced changes in defect-related vibrational features and local bonding. These results demonstrate that nitrogen incorporation and the resulting structural and optical modifications of sputtered AZO films are governed by the combined effects of the initial oxygen partial pressure and subsequent nitridation conditions, providing a basis for controlling AZO properties for optoelectronic and sensing applications. This study provides a foundation for tailoring AZO surface chemistry and defect structure, supporting the future development of films with improved functionality for gas-sensing and optoelectronic applications.

**Keywords:** Aluminum doped zinc oxide, Post-Thermal Nitridation, Nitrogen Doping, Optical and Surface Properties

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