

Supporting Information:

Enhanced Conductivity and Microstructure in Highly Textured $TiN_{1-x}/c-Al_2O_3$ Thin Films

Alexander Zintler¹, Robert Eilhardt¹, Stefan Petzold², Sankaramangalam Ulhas Sharath², Enrico Bruder³, Nico Kaiser², Lambert Alff² & Leopoldo Molina-Luna^{1,}*

¹ Advanced Electron Microscopy, Institute of Materials Science, TU Darmstadt, Alarich-Weiss-Str. 2, 64287 Darmstadt, Germany

² Advanced Thin Film Technology, Institute of Materials Science, TU Darmstadt, Alarich-Weiss-Str. 2, 64287 Darmstadt, Germany

³ Physical Metallurgy, Institute of Materials Science, TU Darmstadt, Alarich-Weiss-Straße 2, 64287 Darmstadt, Germany

Keywords: titanium nitride, thin film electrodes, superconductivity, scanning transmission electron microscopy, grain boundary dissociation

*Corresponding author e-mail: leopoldo.molina-luna@aem.tu-darmstadt.de

This is open-access material distributed under the terms of the Creative Commons Attribution-NonCommercial-NoDerivatives 4.0 International (CC BY-NC-ND 4.0)
<https://creativecommons.org/licenses/by-nc-nd/4.0/>

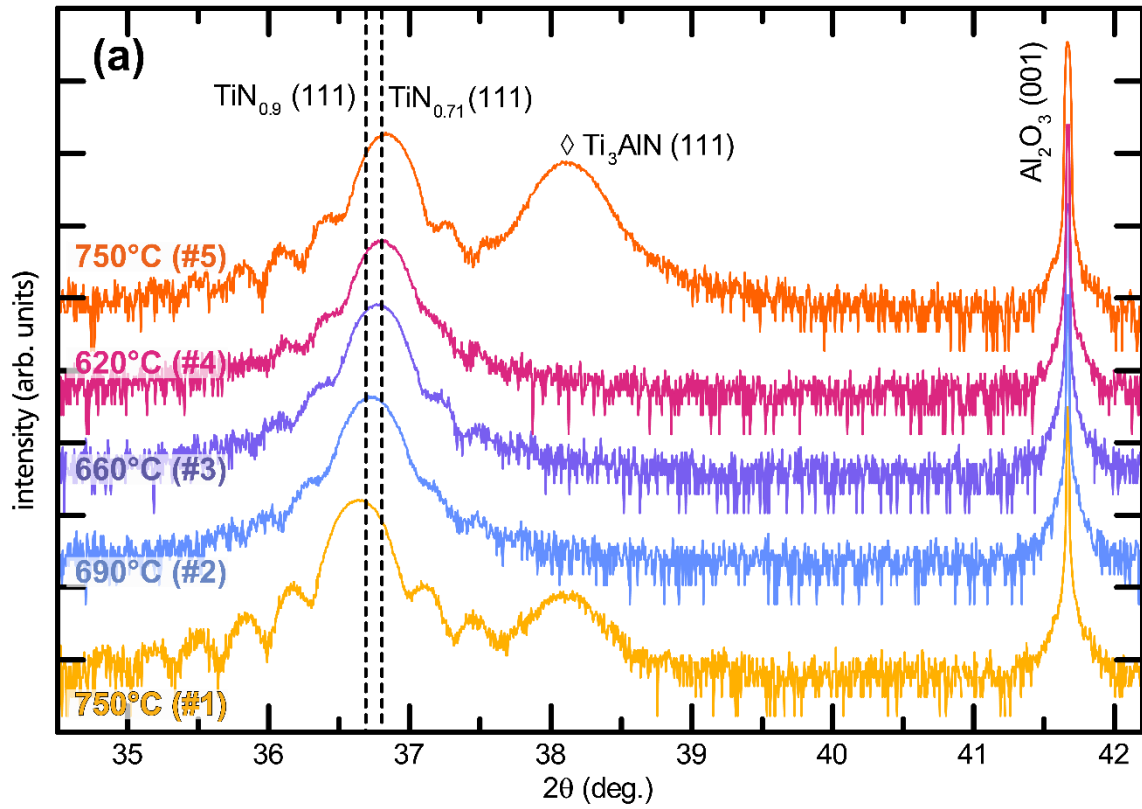


Figure S 1: As shown by the X-ray diffraction patterns, for a Ti evaporation rate of 0.2 Å/s, the TiN (111) peak shifts towards lower 2θ values with an increase in growth temperature. For $T_{\text{growth}} = 750^\circ\text{C}$ an additional Ti₃AlN (111) peak is observed.

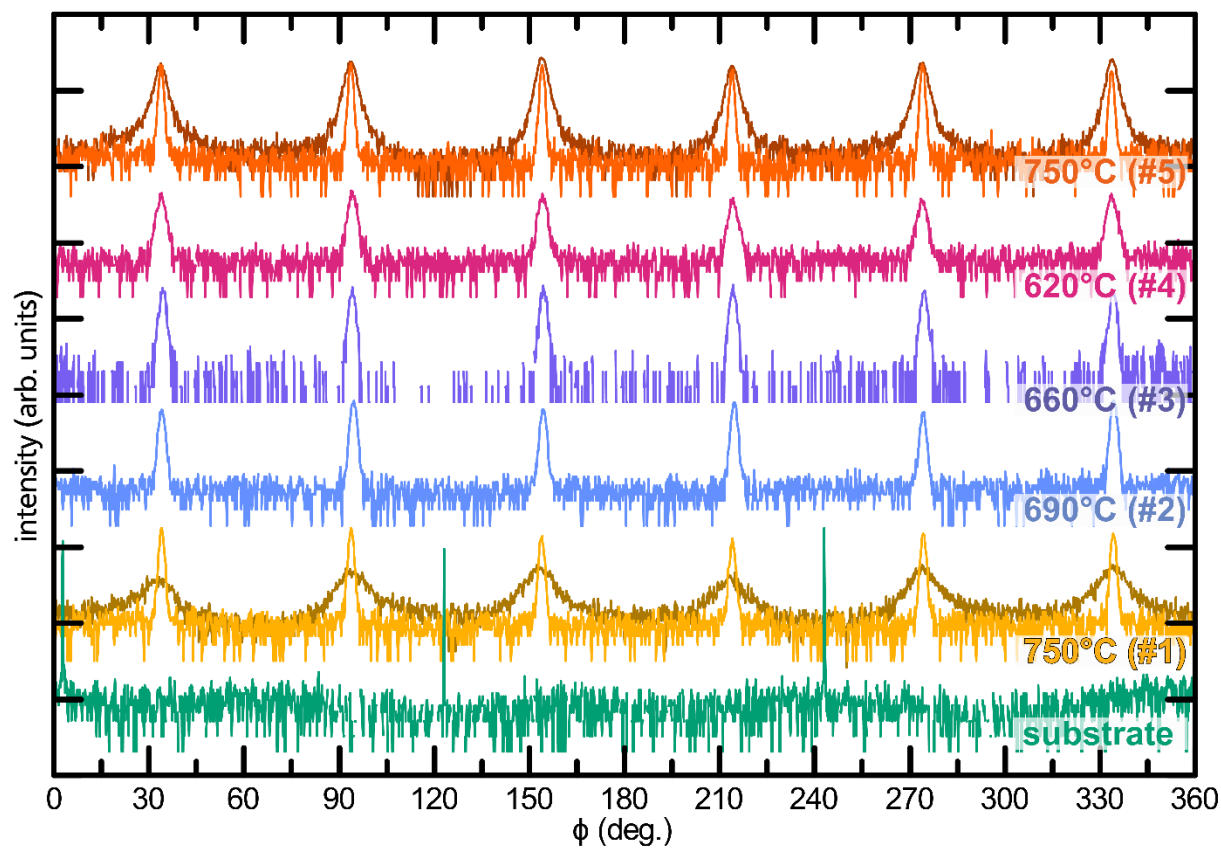


Figure S 2: ϕ -scans indicating two in-plane rotations of the TiN (111) out-of-plane oriented grains, note the 60° separation of the three-fold symmetric {111} peak. The substrate Al_2O_3 (102) ϕ -scan is also displayed (green), which allows to correlate the TiN in-plane rotation to the substrate.

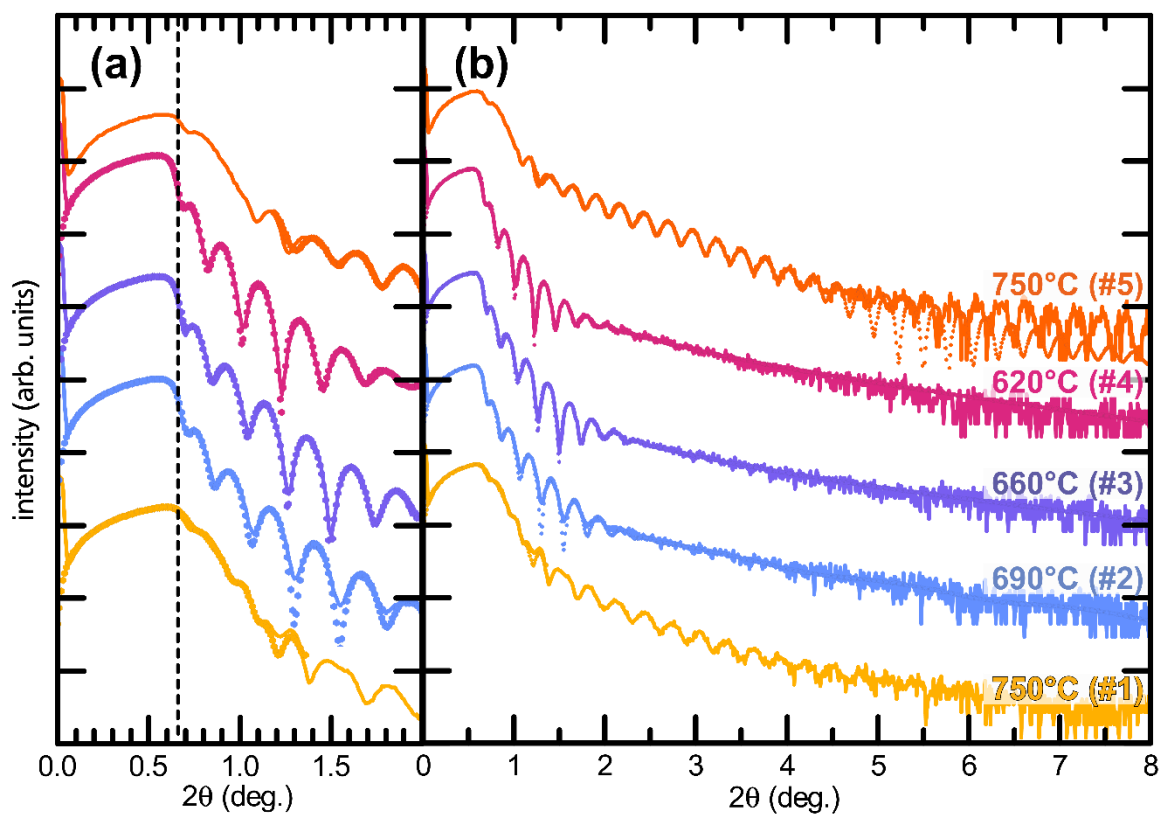


Figure S 3: (a) The critical angle, as shown by the XRR curves, shifts towards higher 2θ values with increased growth temperature for a Ti evaporation rate of 0.2 \AA/s , due to an increase in density of the thin film. (b) The XRR oscillations are dampened for the samples #2-4.

The change in stoichiometry as a function of growth temperature can also be observed in the XRR curves (Figure S 3a) by a shift of the critical angle towards higher 2θ values, indicating an increase in film density. The XRR curves of the samples grown between 620°C and 690°C (pink, purple, blue) show no oscillations at a 2θ value larger than 2° , due to the high surface roughness (Figure S 3b). For the samples grown at 750°C (orange, yellow), the formation of new phases near the substrate interface can be associated with a dampening of the XRR curve oscillations. Nonetheless, the oscillations are still present at high 2θ angles of 5° , indicating a smooth surface.

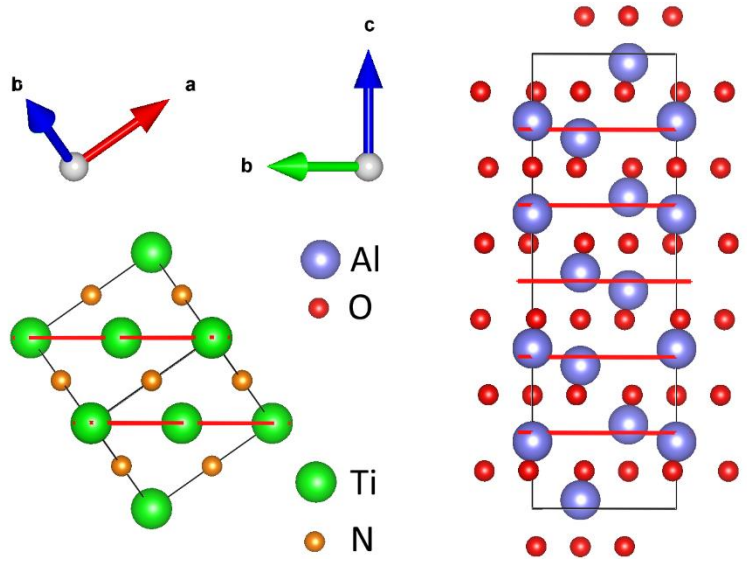


Figure S 4: TiN (left) and Al₂O₃ (right) unit cells with their (111) and (001) facing upwards (growth direction). Red lines denote the (111) and $c/6$ lattice planes respectively.