Supplementary Information (SI) for Nanoscale.
This journal is © The Royal Society of Chemistry 2025

Supporting Information

Effects of Crystal Orientations on Oxidation of Epitaxial TiN Thin Films

Zi-Qin Wang[a,b], Wen-Wen Fan[a,b], Yu-Hong Li[a,b], Hua-Long Zhu[a,b], Yu-Jia Wang[a,b], Yun-Long Tang[a,b*]

[a]Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China

[b]School of Materials Science and Engineering, University of Science and Technology of China, Shenyang 110016, China

*Correspondence: Y.-L. T. (yltang@imr.ac.cn)

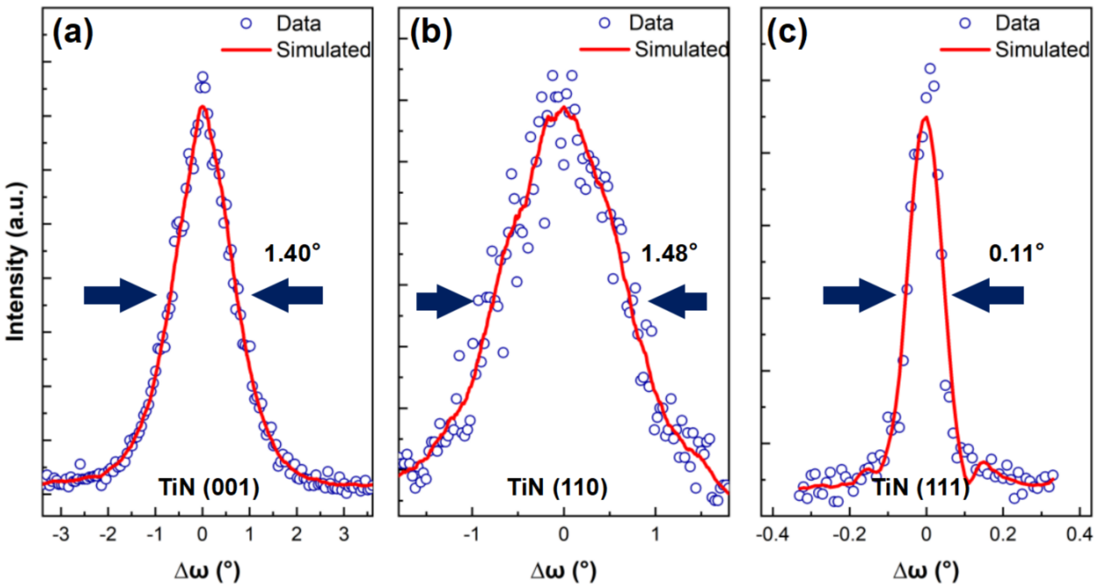

Figure S1 The rocking curves of the [001]-, [110]-, and [111]-oriented epitaxial TiN thin films around (113), (222), and (113) diffractions.

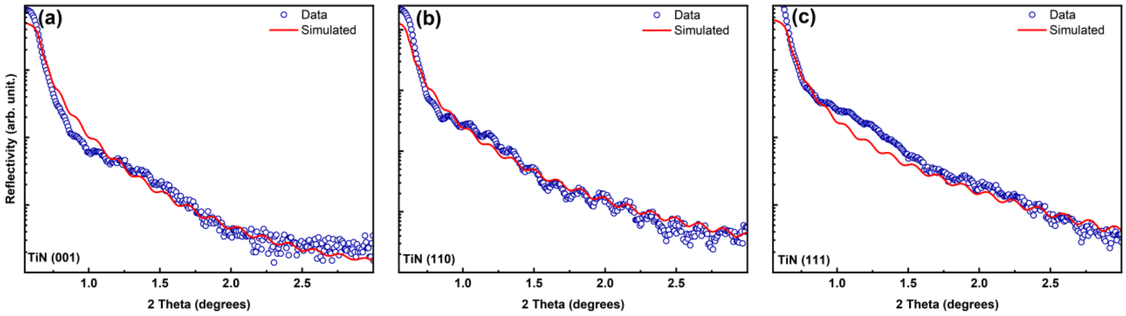

Figure S2 The XRR scan of the TiN thin films together with the best-fit scan (red line) obtained using Parrat's formalism.

Table S1 Thickness, roughness, and density of [001]-, [110]-, and [111]-oriented epitaxial TiN thin films.

Orientation	Thickness (nm)	Roughness (nm)	Density (g/cm^3)
[001]	47.706	0.362	5.289
[110]	50.879	0.372	4.660
[111]	47.557	0.604	5.320

The thickness of the [001]-, [110]-, and [111]-oriented epitaxial TiN thin films, that was estimated from XRR data shown in Figure S1, was 47.706 nm, 50.879 nm, and 47.557 nm, respectively. The detailed information on roughness and density of the [001]-, [110]-, and [111]-oriented epitaxial TiN thin films were shown in Table S1. The roughness of the films exhibited an order of [001] < [110] < [111].

The [111]-oriented TiN thin film has shown a narrow rocking curve. The TiN thin films grow preferentially along the [111] direction, and thus the [111]-oriented TiN film tends to have a higher growth quality

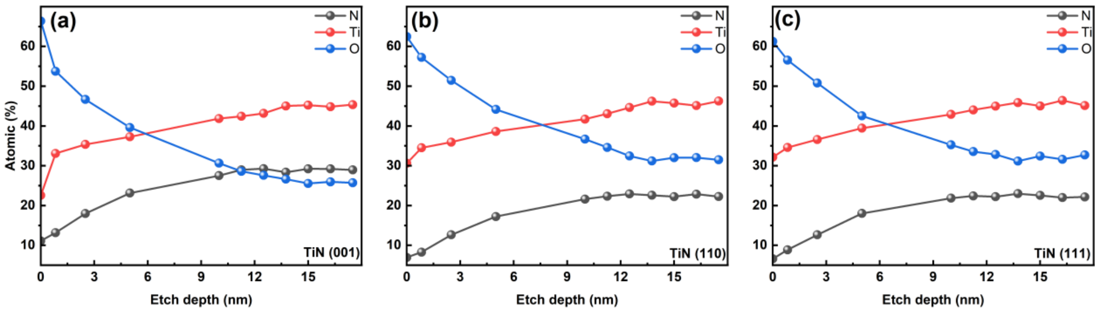

Figure S3 The XPS depth profiling of [001]-, [110]-, and [111]-oriented epitaxial TiN thin films by Ar+ ion etching. The x-axis has converted into film depth.

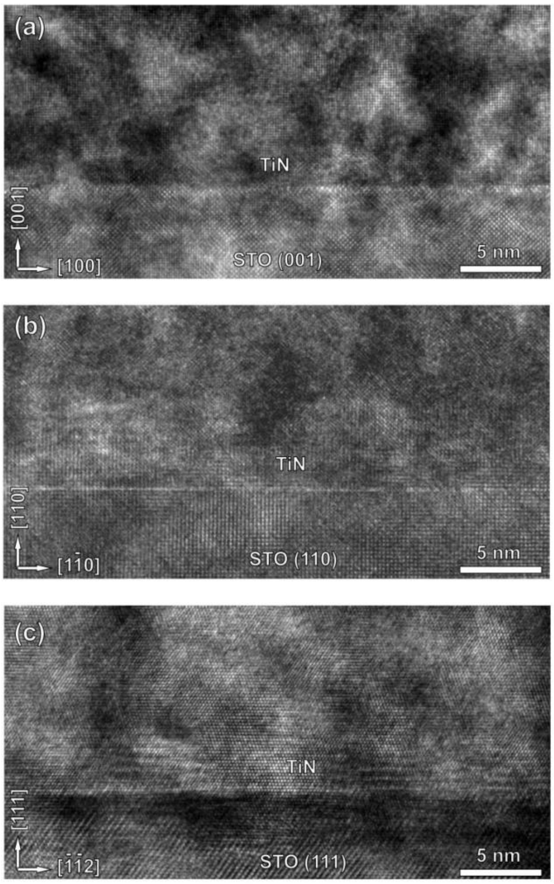

Figure S4 HRTEM images of the [001]-, [110]-, and [111]-oriented epitaxial TiN thin films.

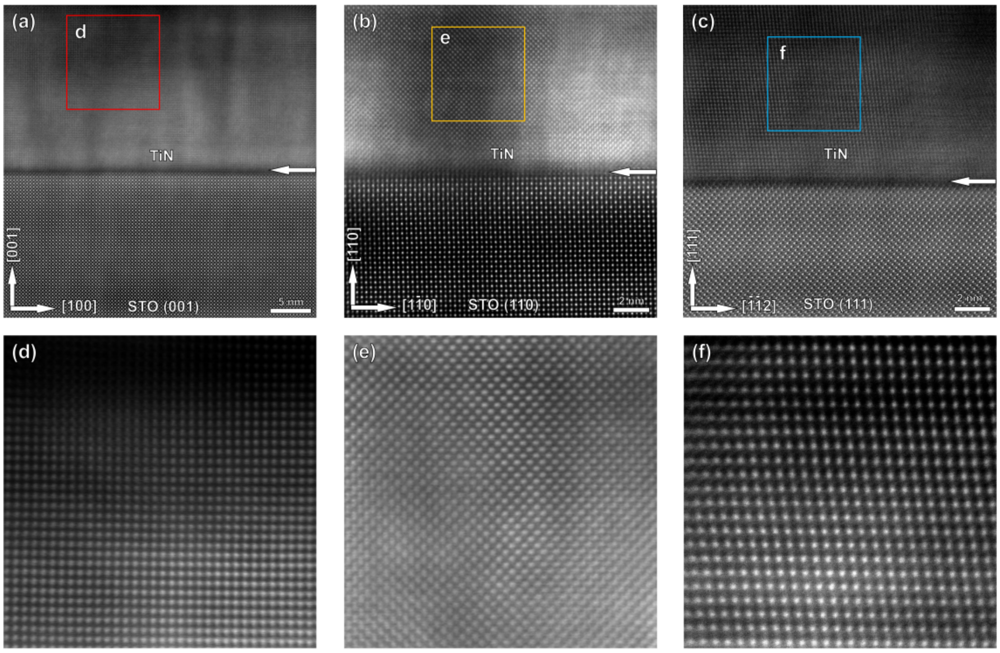

Figure S5 (a-c) HAADF-STEM images of TiN thin films. (d-f) Enlarged atomic-scale HAADF-STEM images of TiN thin films.

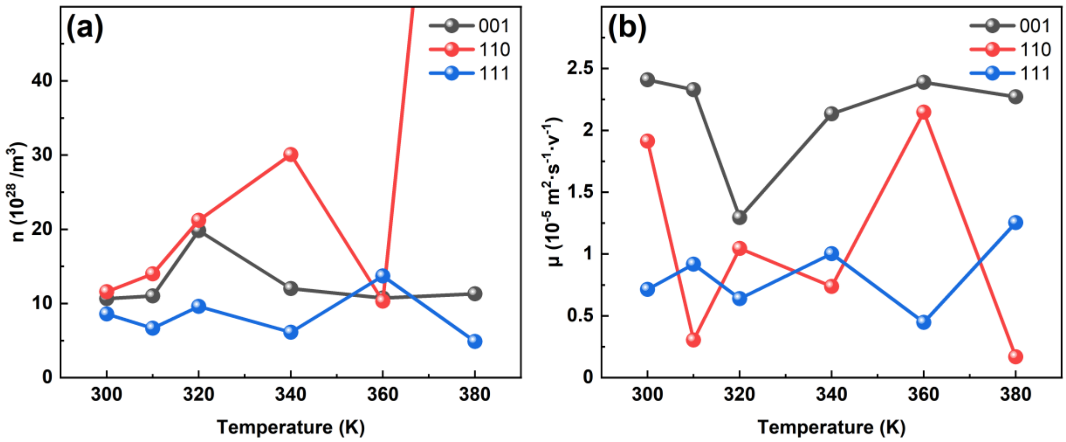

Figure S6 Carrier concentration n and carrier mobility μ of the [001]-, [110]-, and [111]-oriented epitaxial TiN thin films by physical property measurement system in the temperature range 300-380 K.