

SUPPLEMENTARY INFORMATION

Thermoelectric and Electronic Transport Properties of Thermal and Plasma-Enhanced ALD Grown Titanium Nitride Thin Films

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Table S1: Selected Area electron diffraction measurements. The radius was measured using ImageJ software.

TiN crystal orientations	Radius (nm)-PEALD	Radius (nm)-Thermal ALD
[111]	4.25±0.2	4.77±0.03
[200]	5.01±0.01	5.15±0.1
[220]	7.110±0.1	7.52±0.4
[311]	10.84±0.1	11.34±0.1

d-spacing for the diffraction planes were measured from radius using formula, $d = 1/\text{radius}$. This d-spacing is then used for indexing rings.

Table S2: Variation of the thermoelectric properties of PEALD TiN thin films grown at different temperature

Growth temp (C)	Thickness TiN(nm)	Seebeck coefficient (μV/K)	Conductivity $\times 10^4$ (Sm ⁻¹)	PF (μW/mK ²)	Hall mobility (cm ² /Vs)	Carrier density (cm ⁻³)	Resistivity $\times 10^{-4}$ (Ω cm)
200°	20±3	- 23.6±0.003	3.37±2.3	18.1±0.8	0.032±0.002	2.59 $\times 10^{22}$	29.7
300°	31±2,7	- 21.0±0.001	32±0.1	137±3	0.41±0.02	3.3 $\times 10^{22}$	3.13
400°	31±2	- 20.2±0.002	116±3.3	437±4	0.78±0.04	4.86 $\times 10^{22}$	0.91

Table S3: Variation of the thermoelectric properties of thermal ALD TiN thin films grown at different temperature

Growth temp (C)	Thickness TiN(nm)	Seebeck coefficient (μV/K)	Conductivity $\times 10^4$ (Sm ⁻¹)	PF (μW/mK ²)	Hall mobility (cm ² /Vs)	Carrier density (cm ⁻³)	Resistivity (Ω cm)
200°	No growth	-	-	-	-	-	-
300°	1.2 ±0.8	-	-	-	-	-	-
400°	12.0±2	-702±0.007	2.4±0.02	1.18±0.1	2±0.02	7.59 $\times 10^{20}$	41.7±2

Table S4: Variation of the thermoelectric properties of PEALD TiN thin films grown at 400°C with number of ALD cycles

No. of cycles	Thickness TiN(nm)	Seebeck coefficient ($\mu\text{V/K}$)	Conductivity $\times 10^4$ (S m^{-1})	PF ($\mu\text{W/mK}^2$)	Hall mobility (cm^2/Vs)	Carrier density (cm^{-3})	Resistivity $\times 10^{-5}$ ($\Omega \text{ cm}$)
600	17.7 $\pm$ 3	-19.4 $\pm$ 0.3	63.6 $\pm$ 2.3	18.4 $\pm$ 0.8	0.45 $\pm$ 0.002	5.59 $\times 10^{22}$	16
1200	31 $\pm$ 2	-20.2 $\pm$ 0.002	116 $\pm$ 3.3	437 $\pm$ 4	0.78 $\pm$ 0.04	4.86 $\times 10^{22}$	8.6
2000	50.4 $\pm$ 1.5	-23.4 $\pm$ 0.2	120 $\pm$ 2	512 $\pm$ 4	1.5 $\pm$ 0.04	2.81 $\times 10^{22}$	8.3

Table S5: Variation of the thermoelectric properties of thermal ALD TiN thin films grown at 400°C with number of ALD cycles

No. of cycles	Thickness TiN(nm)	Seebeck coefficient ($\mu\text{V/K}$)	Conductivity (S m^{-1})	PF ($\mu\text{W/mK}^2$)	Hall mobility (cm^2/Vs)	Carrier density (cm^{-3})	Resistivity ($\Omega \text{ cm}$)
600	5.8	-	-	-	0.4 $\pm$ 0.002	12 $\times 10^{20}$	-
1200	12 $\pm$ 2	-702 $\pm$ 0.007	2.4 $\pm$ 0.02	1.18 $\pm$ 0.1	2 $\pm$ 0.02	7.59 $\times 10^{20}$	42 $\pm$ 1
2000	24.1 $\pm$ 0.7	-74.3.4 $\pm$ 0.7	935 $\pm$ 3.3	4.95 $\pm$ 0.2	33 $\pm$ 0.02	0.22 $\times 10^{20}$	0.11 $\pm$ 0.02

Figure S1: HRTEM images confirming the thickness of thermal ALD and PEALD TiN grown with 1200 cycles at 400°C

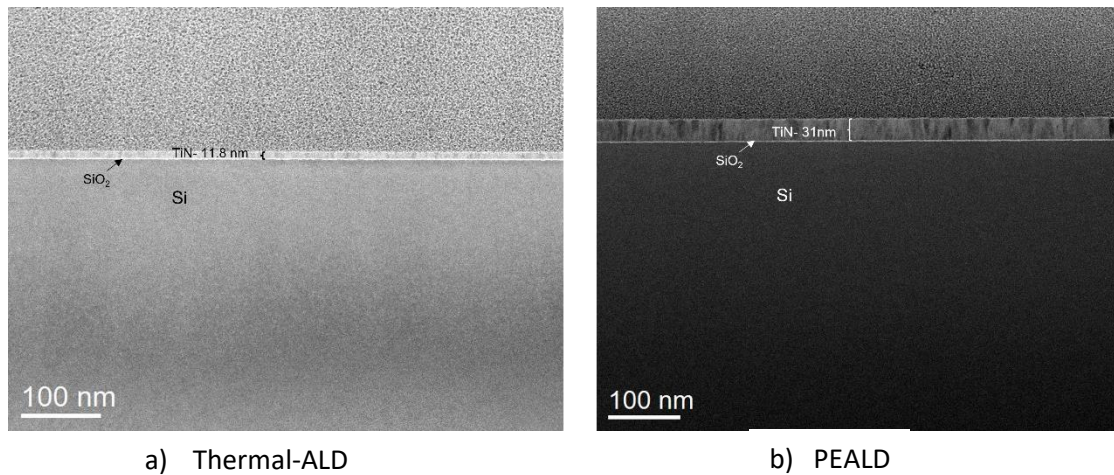


Table S6: Other details of the PEALD TiN sample used for fitting the model:

Material	Thickness (nm)	Cp (J/kgK)	rho (kg/dm^3)	K (W/mK)
Au	176,00	129,00	19,30	317,00
Ti	17,00	522,00	4,51	21,90
Si	500000,00	703,00	2,34	150,00

Density (TiN): 5,40 kg/dm³

Specific heat capacity for TiN: 636,00 J/kgK

For PEALD TiN Film-

Thermal Conductivity (W/m·K) after fitting: 26.96

Film Thickness (nm): 86.00

R² Value: 0.953935

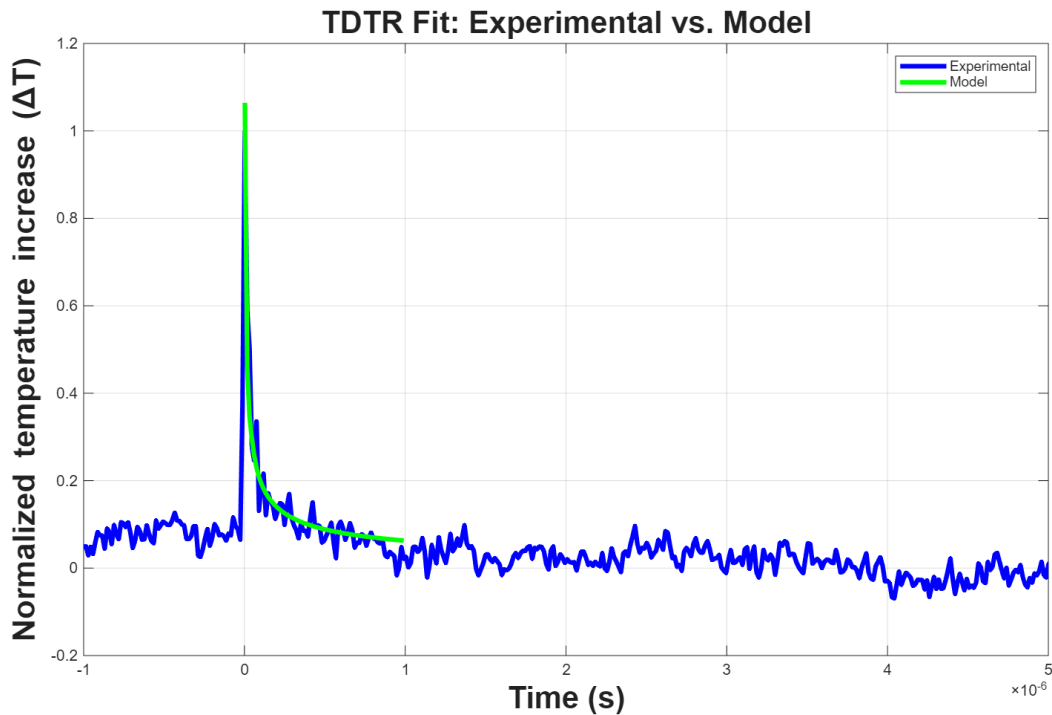


Figure S2: Thermal Conductivity decay curve for PEALD TiN after fitting

For thermal ALD TiN Film-

Thermal Conductivity (W/m·K) after fitting: 7.01

Film Thickness (nm): 86.5

R² Value: 0.97

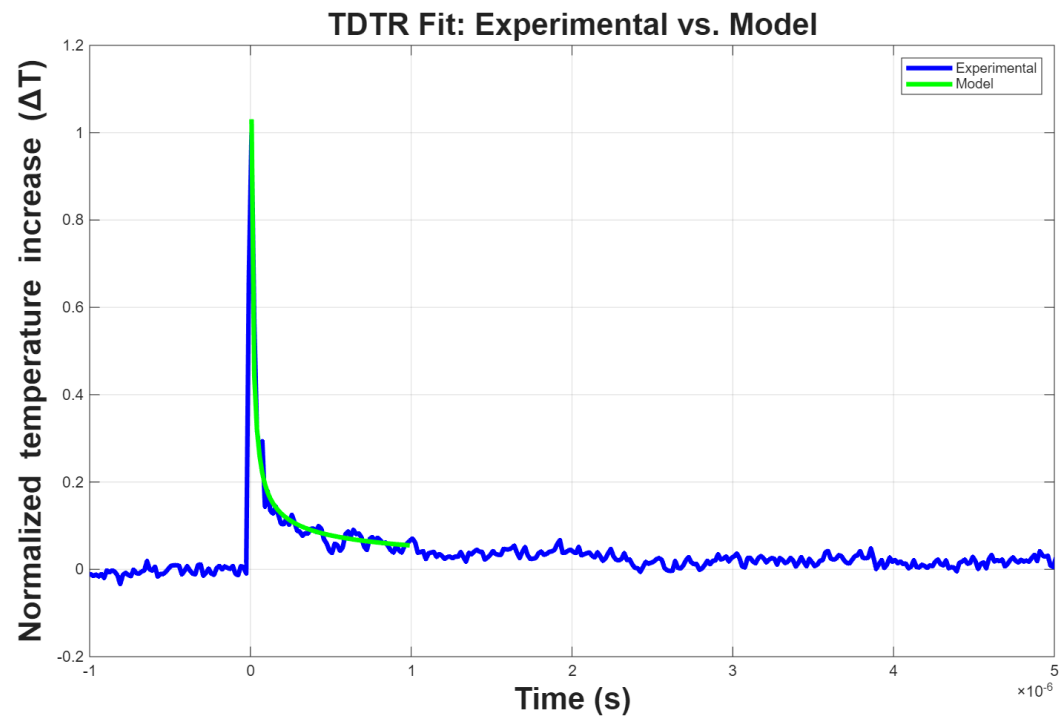


Figure S3: Thermal Conductivity decay curve for thermal ALD TiN