Structural, Optical and Photoelectrochemical Characterizations of Monoclinic Ta_3N_5 Thin Films

Sherdil Khan[a], Maximiliano J. M. Zapata[a], Marcelo B. Pereira[a], Renato V. Gonçalves[b], Lukas Strizik[d], Jairton Dupont[e], Marcos J. L. Santos[c], Sérgio R. Teixeira[a*]

a. Institute of Physics, Universidade Federal do Rio Grande do Sul, Av Bento Goncalves 9500 POBox - 15051 91501-970, POA-RS, Brazil

b. Instituto de Física de São Carlos, Universidade de São Paulo, CP 369, São Carlos 13560–970, SP, Brazil

c. Institute of Chemistry, Universidade Federal do Rio Grande do Sul, Av Bento Goncalves 9500, POA-RS, Brazil

d. Department of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, Studentska 573, 53210, Pardubice, Czech Republic.

e. School of Chemistry, University of Nottingham, University Park, Nottingham, NG7 2RD, United Kingdom.

email: * srgrbrtxr@gmail.com

†Supplementary Information

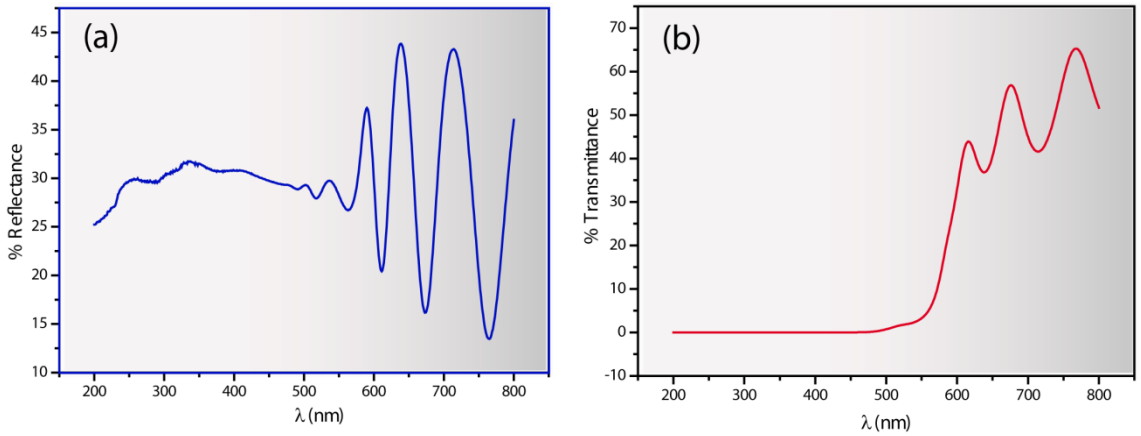

Fig. S1 UV-Vis (a) Reflectance and (b) Transmittance spectra of Ta_3N_5 thin films.

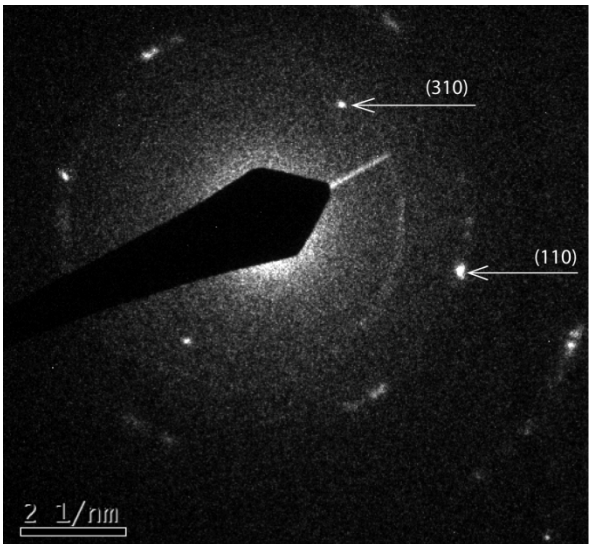

Fig. S2 SAED pattern of monoclinic Ta_3N_5 thin film.

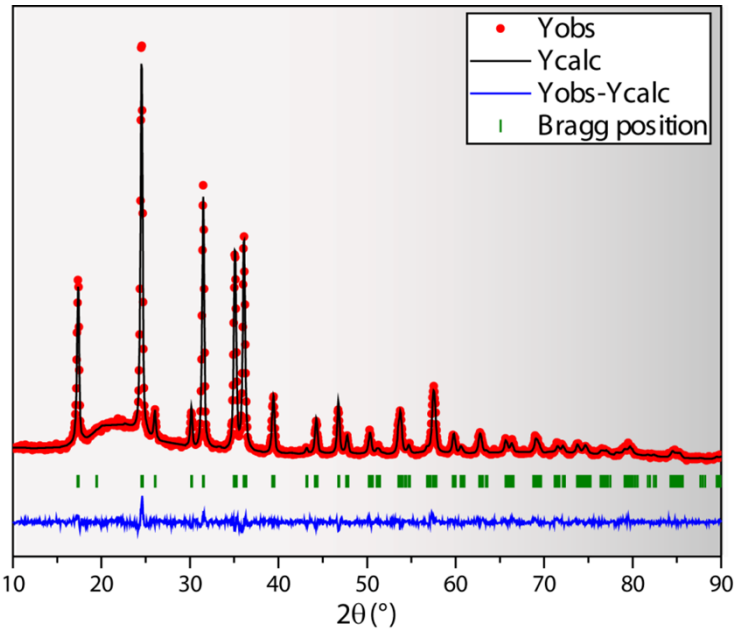

Fig. S3 Rietveld refinement fitting curves.

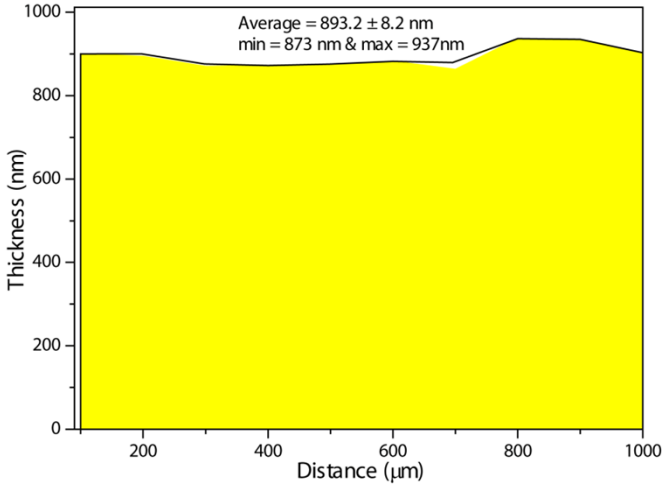

Fig. S4 Profilometry of Ta_3N_5 thin film.

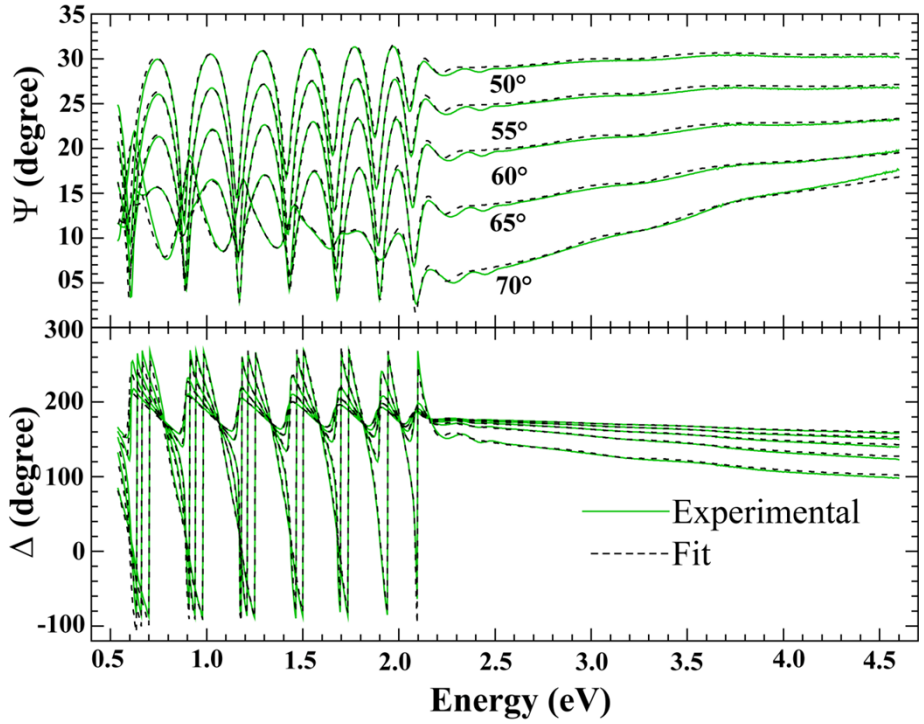

Fig. S5 The experimental SE parameters Ψ and Δ (green lines) fitted by the model (black dashed lines).

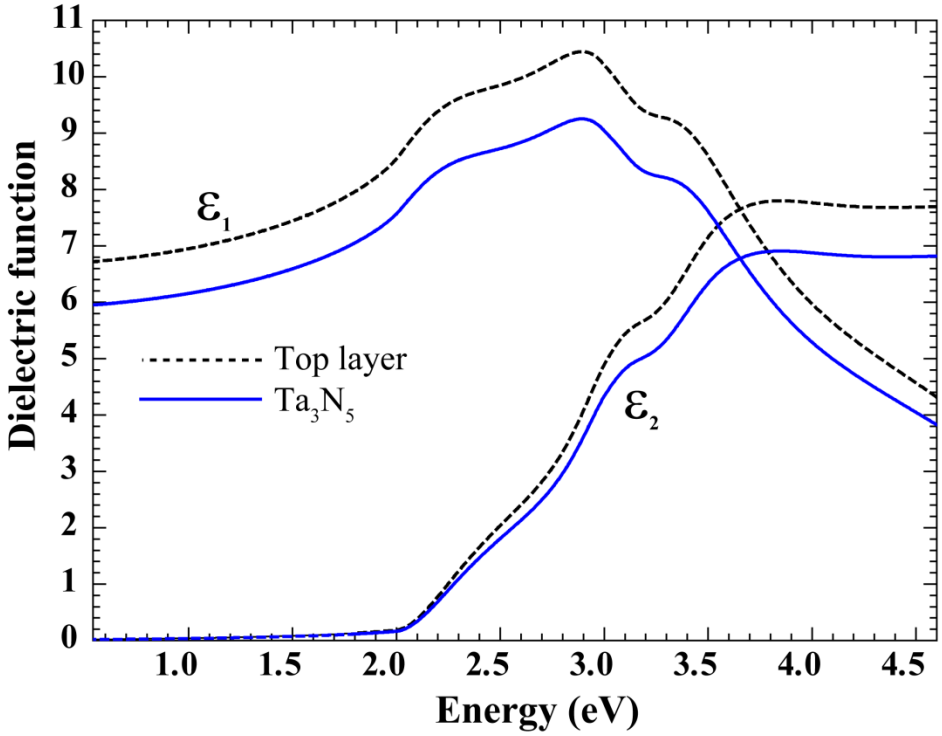

Fig. S6 Real ε_1 and imaginary ε_2 parts of dielectric functions for top layer and sub-top layer obtained by the SE analyses.

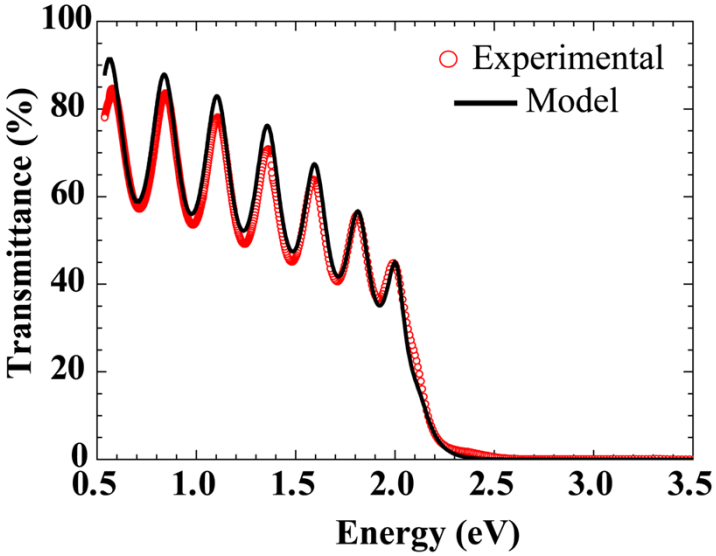

Fig. S7 Transmittance of the Ta_3N_5 films calculated from the parameterization of the SE data (black line) and experimentally measured by the UV-Vis-NIR spectroscopy (red circles).

Table. S1The bond distances (Å), average grain size and grain size as a function of (hkl) (nm) obtained from Rietveld refinement.

Bond distances (Å)					
Size (nm)					
Average	h00	0k0	00l	hk0	0kl
40.428	38.215	38.193	44.725	38.196	38.906

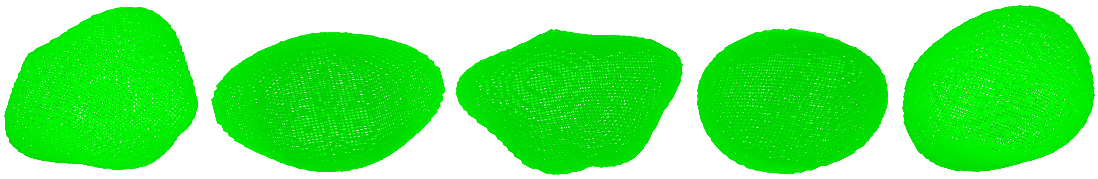

Table. S2 The atomic sites and their %occupancies and %vacancies obtained by Rietveld refinement of Ta_3N_5*

Atom	Wyckoff Position	*x*	*y*	*z*	Site occupancy (%)	Site vacancy (%)
Ta1	4i	0.18857	0.00000	0.25000	99.18	0.82
Ta2	4i	0.13462	0.00000	0.56330	100.00	0.00
Ta3	4i	0.12534	0.00000	0.93594	100.00	0.00
N1	4i	0.75000	0.00000	0.25000	96.95	3.05
N2	4i	0.09349	0.00000	0.06327	**98.72**	**0.00**
O1		0.03693	0.00000	0.15532	**1.28**	
N3	4i	0.07089	0.00000	0.38304	**90.95**	**0.00**
O2		0.03287	0.00000	0.38067	**9.05**	
N4	4i	0.31792	0.00000	0.04001	100.00	0.00
N5	4i	0.30020	0.00000	0.42430	100.00	0.00

**Space group, C 2/m, a=10.2058Å;b=3.8863Å, c=10.2636Å, α=β=Ɣ=90°*
R_p=3.04;R_{Bragg}=3.10, χ^2 =1.61.