Enhanced performance in transparent conducting materials at the interface of a wide band gap semiconductor and a correlated metal

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Supplementary Information:

AFM

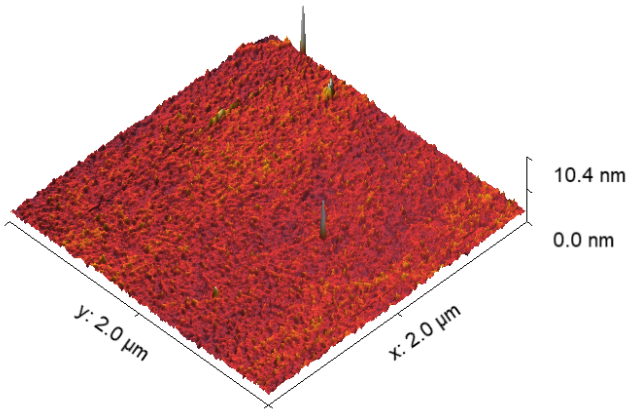


Figure S 1: Morphology of a 17nm $SrNbO_3$ film grown on (0 0 1) $SrTiO_3$ substrate measured using atomic force microscopy

XRR

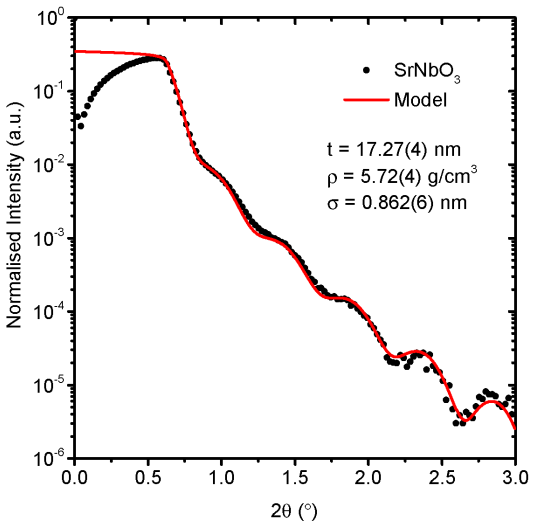


Figure S 2: X-ray reflectivity of a 17nm $SrNbO_3$ thin film

XRD

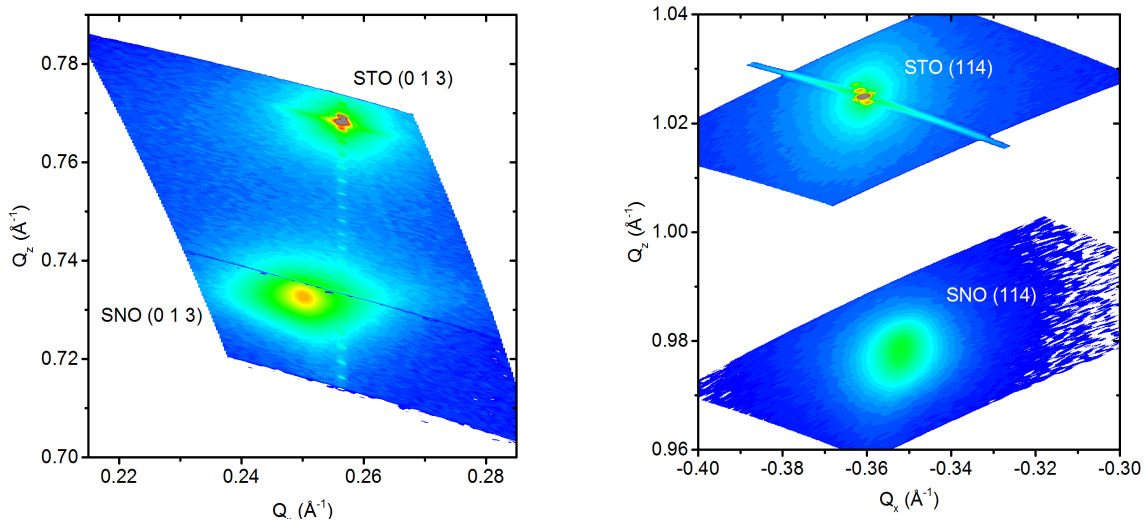


Figure S 3: Reciprocal space maps of a 74 nm $SrNbO_3$ thin film around the (0 1 3) and (1 1 4) reflections

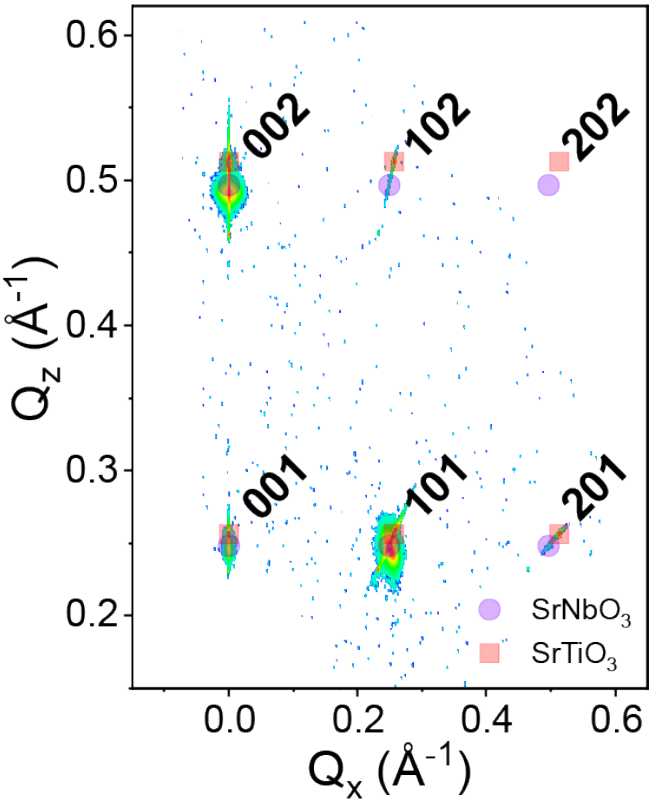


Figure S 4: Wide RSM collected using a 2D Hypix detector

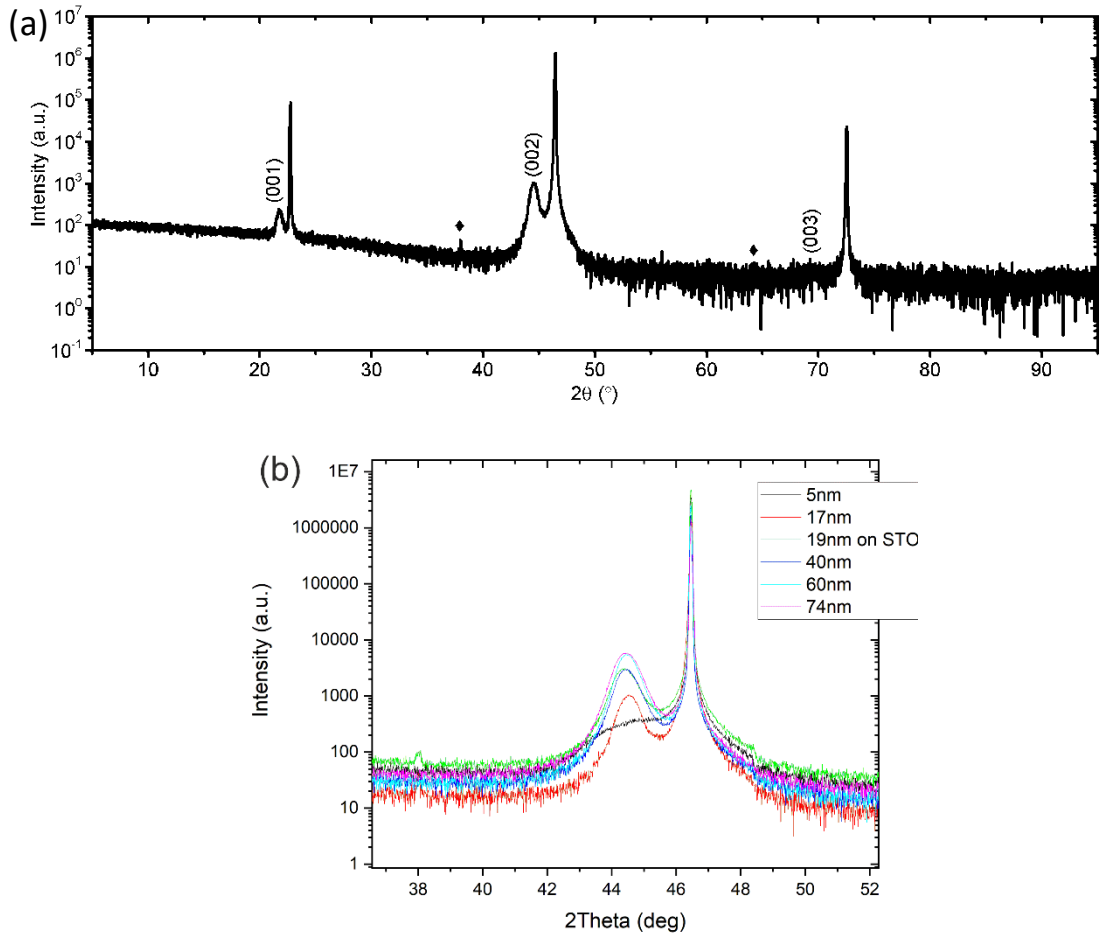


Figure S 6: (a) X-ray diffraction pattern of a 17 nm $SrNbO_3$ thin film, the diamonds correspond to silver paste on the edges of the sample used to attach the substrate to the sample plate during growth (b) X-ray diffraction patterns for various thickness $SrNbO_3$ thin films deposited on $SrTiO_3$ substrate around the 002 peak.

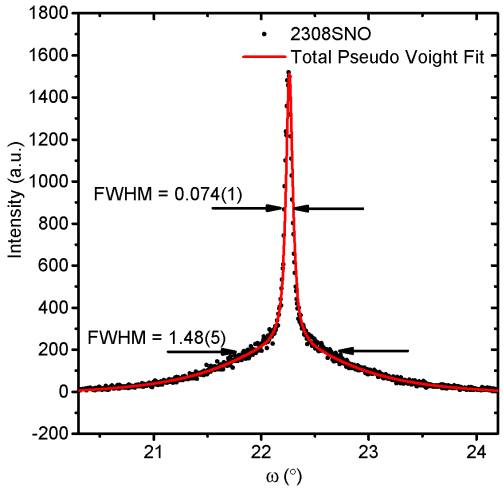


Figure S 5. Rocking curve of the (0 0 2) reflection of a 17 nm $SrNbO_3$ thin film

Additional TEM images

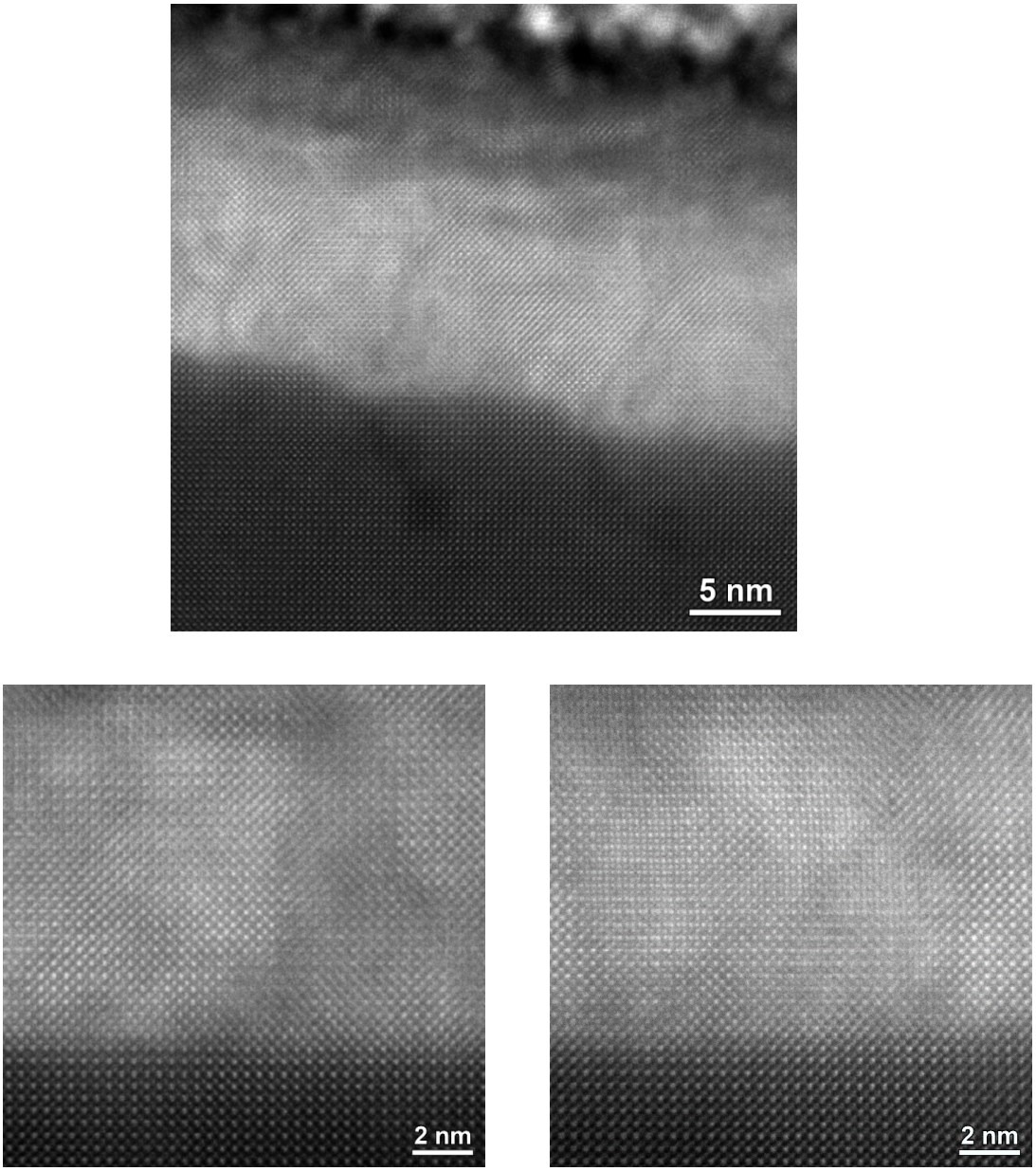
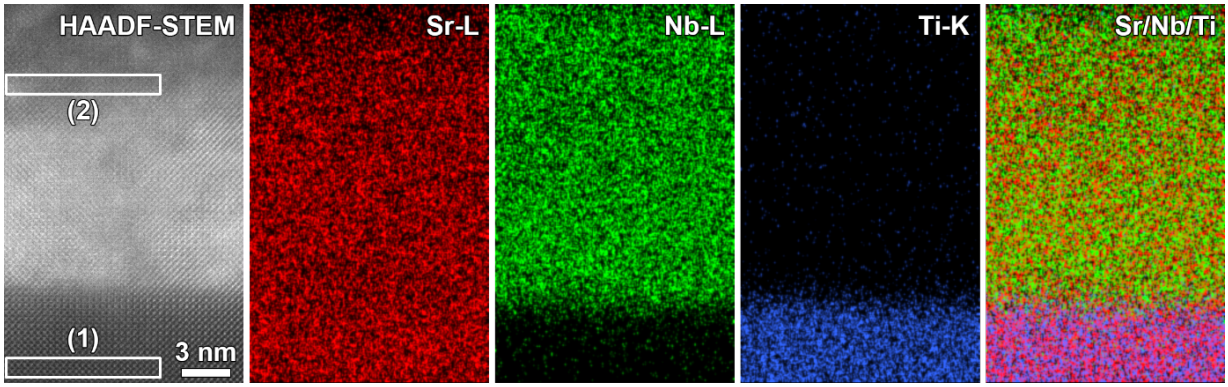
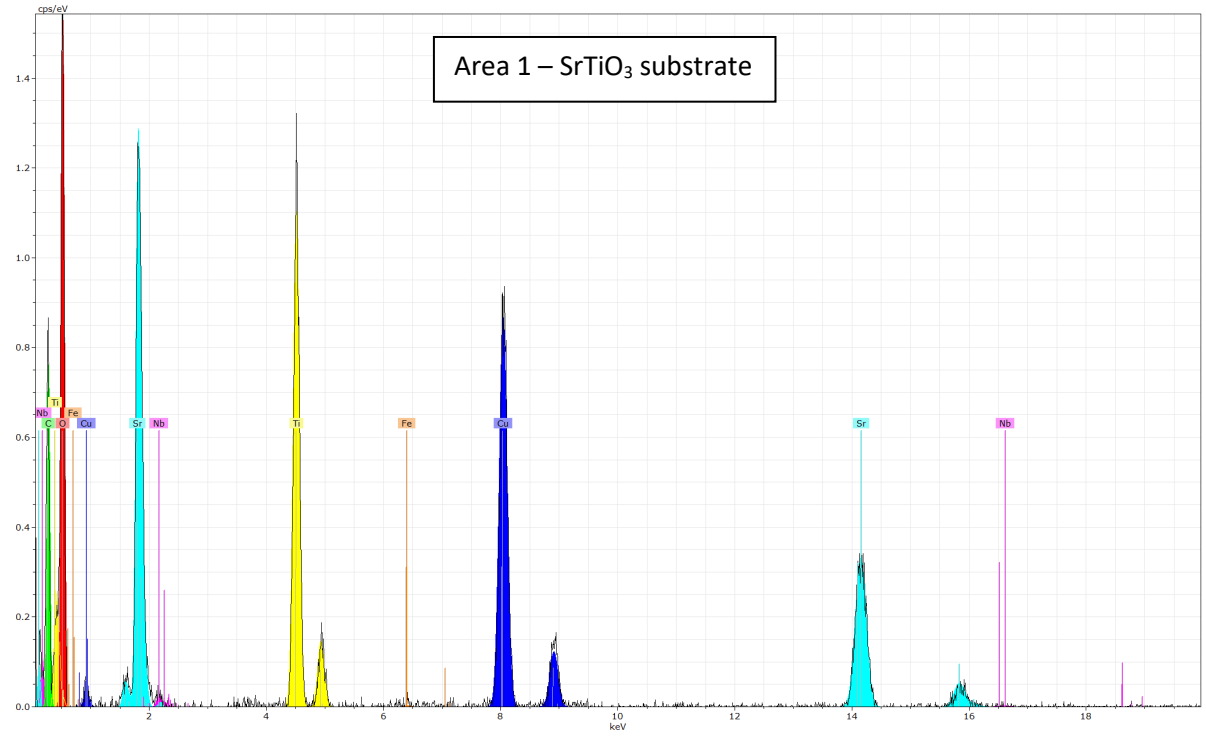


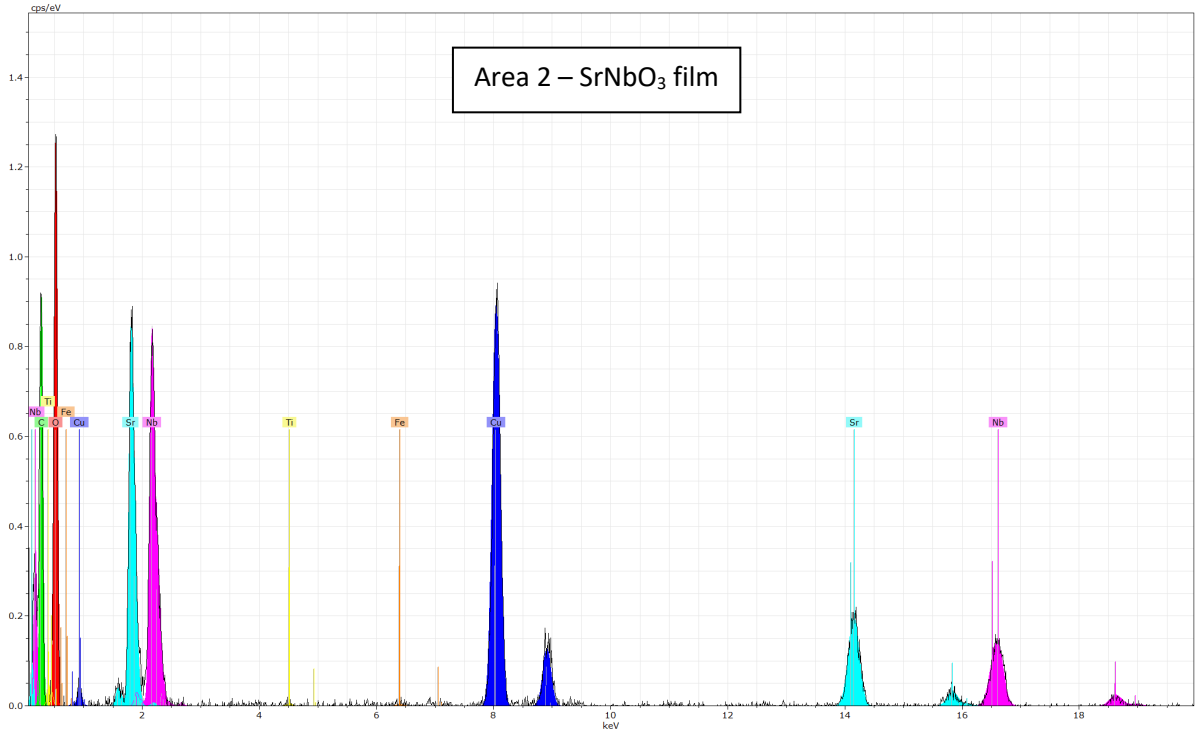
Figure S 7 HAADF-STEM images showing the STO/SNO interface

(a)


HAADF-STEM
(2)
(1)
3 nm
Sr-L
Nb-L
Ti-K
Sr/Nb/Ti

(b)


Area 1 – SrTiO3 substrate
cps/eV
keV
Nb
Ti
Fe
Cr
O
Cu
Sr
Nb
Ti
Fe
Cu
Sr
Nb



(c)

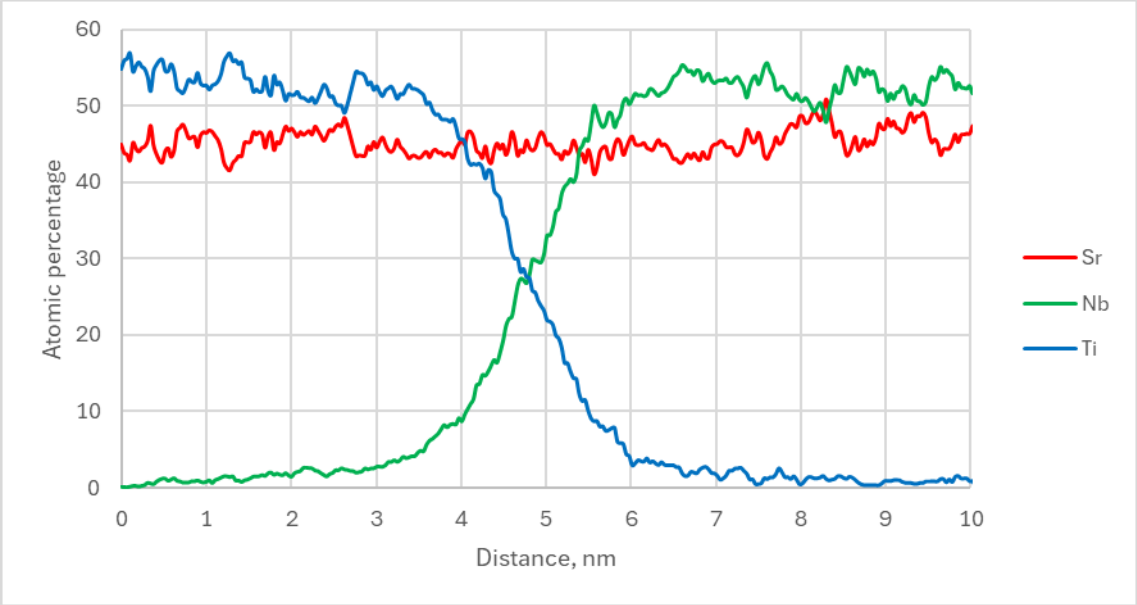
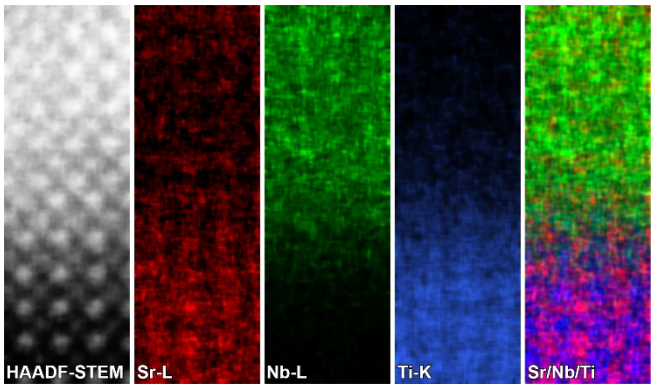


Figure S 8. ***(a)*** *Overview HAADF STEM image and the EDX maps in atomic percent.* ***(b)*** *Deconvoluted EDX spectra acquired far from the interface: (Area 1) STO substrate and (Area 2) SNO film. For the quantification, both K and L lines of Sr and Nb were tested (Sr-K 14.16 keV, Nb-K 16.62 keV, Sr-L 1.81 keV, Nb-L 2.17 keV). L lines gave better result (less deviation and closer to the expected composition) probably because of the closeness to Ti-K line (4.51 keV), so they were used for quantification and mapping. The atomic ration between Sr : Ti : Nb in area (1) 43.9 : 55.1 : 1.0; and in area (2) 47.6 : 0.4 : 52.0. The deviation from an expected composition is related due to the channeling effect [https://doi.org/10.1016/j.ultramic.2014.11.029]. Small signal of Nb in STO layer and Ti in SNO layer is within the error margin.* ***(c)*** *EDX profile measured perpendicular from the STO substrate up to the SNO film and averaged to the whole area. The profile shows that the Ti/Nb mixing occurs within a range of about 2 nm, however it can deviate from area to area.*

(a)



(b)

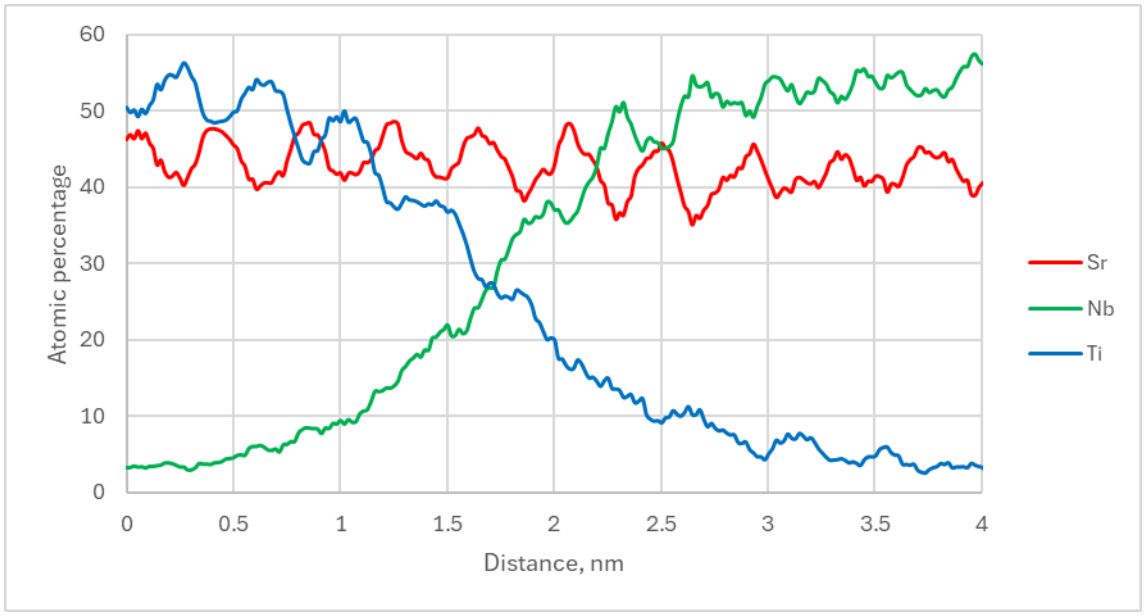


Figure S 9. ***(a)*** *High magnification (5.1 Mx) HAADF STEM image and the EDX maps in atomic percent.* ***(b)*** *EDX profile measured perpendicular from the STO substrate up to the SNO film and averaged to the whole area. The profile shows that the Ti/Nb mixing occurs within a range of about 1-1.5 nm and goes gradually.*

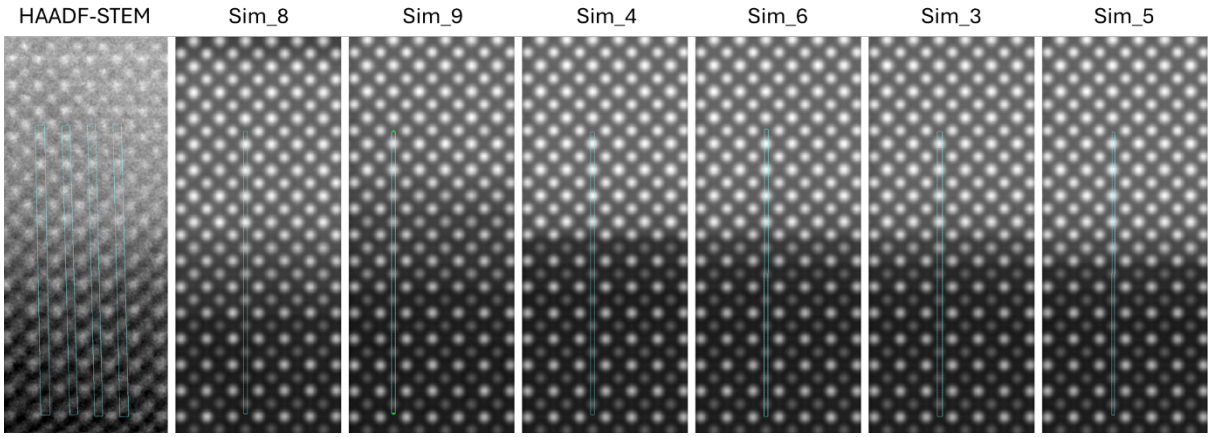


Figure S 10. Experimental HAADF-STEM image and simulations of the interface. Blue lines indicate rows of B cations along which the intensity profiles were measured (see Figure S 8). According to the experimental image, there is a gradual change of the intensity from STO to SNO. The Ti/Nb mixing occurs within a range of about 1.5 nm and occurs gradually. The following models were used for the simulations: (Sim_8) Interface of the three unit cells of Nb/Ti cation mixing with a gradual distribution; (Sim_9) Interface of the four unit cells of Nb/Ti cation mixing with a gradual distribution. The other models correspond to the interfaces of one atomic layer with different Nb/Ti content: (Sim_4) sharp interface without Ti/Nb mixing; (Sim_6) 0.3Nb+0.7Ti; (Sim_3) 0.5Nb+0.5Ti; (Sim_5) 0.7Nb+0.3Ti.

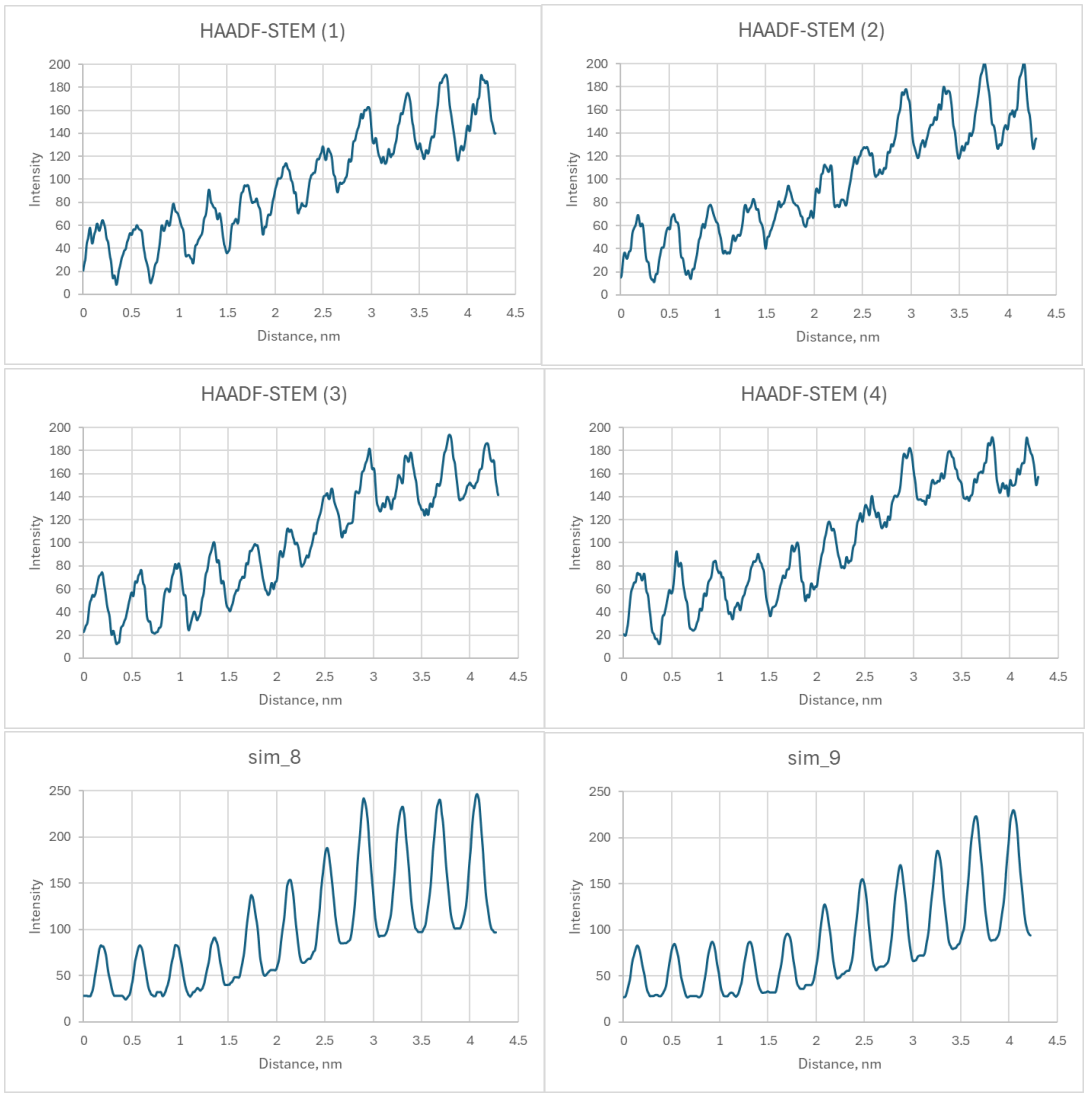


Figure S 11. HAADF-STEM measured intensity profiles (HAADF-STEM1, HAADF-STEM2, HAADF-STEM3. HAADF-STEM4), corresponding to the blue lines in Figure S 7 and simulated (bottom) intensity across the interface with SIM8: three unit cells of Nb/Ti cation mixing with a gradual distribution and SIM9: 4 atomic layers with gradual Ti/Nb distribution.

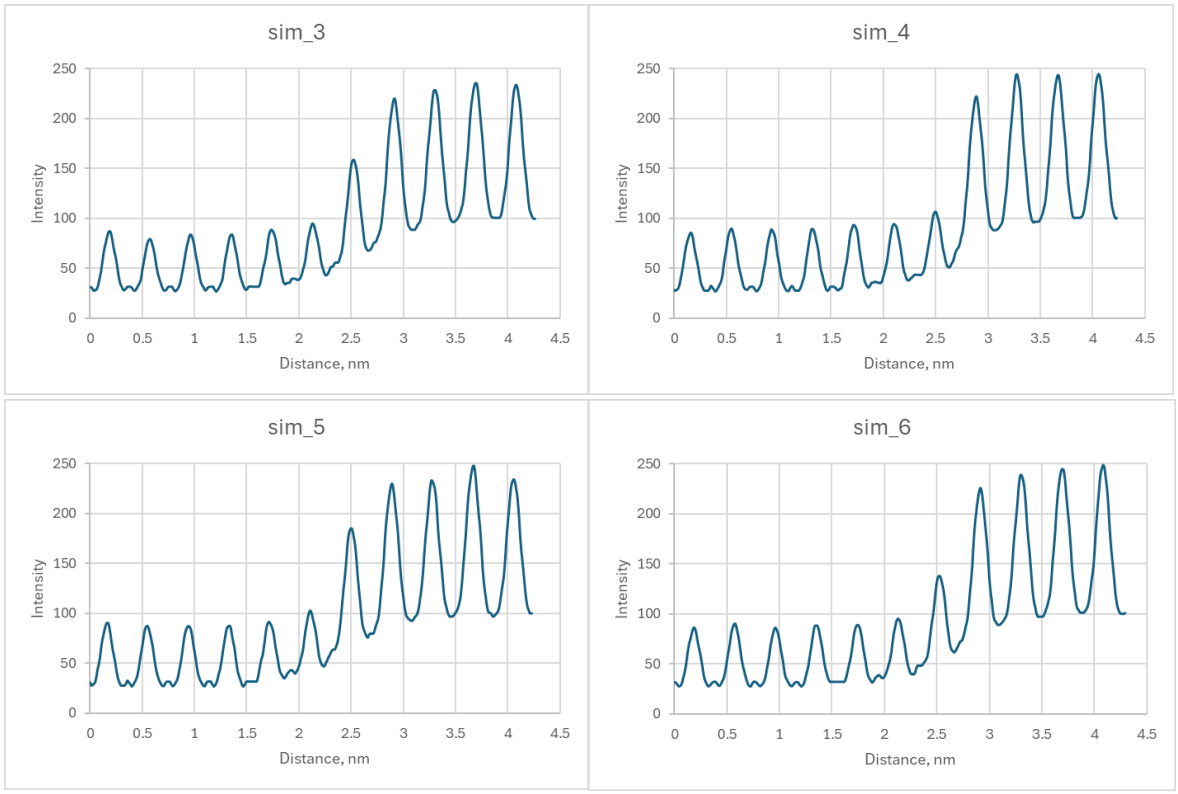


Figure S 12 Alternative simulated HAADF-STEM intensity profiles modelled with the interface one atomic layer thick. Sim3: 0.5Nb+0.5Ti, SIM4: sharp interface with no mixing; SIM5: 0.7Nb+0.3Ti; SIM6: 0.3Nb+0.7Ti;

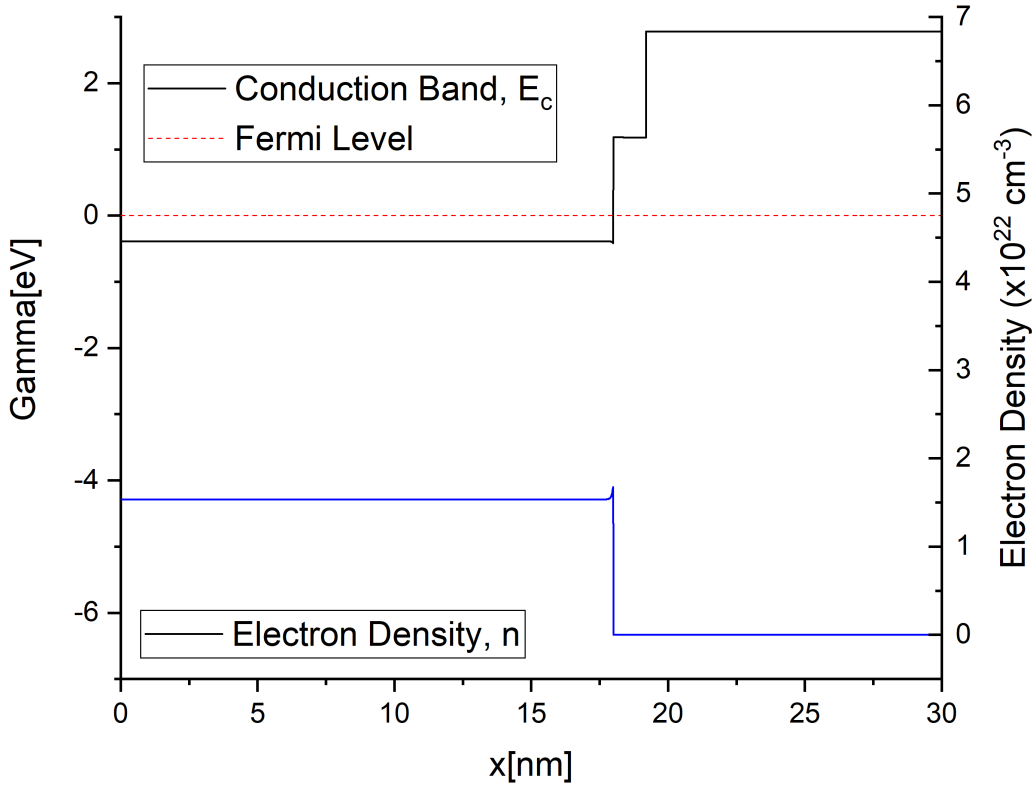


Figure S 13. Poisson solution of the conduction band, Ec (black) and the electron density (blue) for a SrTiO3/SrNbxTi1 xO3/SrTiO3(substrate) system, where x = 0.5 over 1.2 nm (i.e. 3 unit-cells of SrNbO3). The Fermi level is indicated by the red dotted line.

XANES Absorption Edge

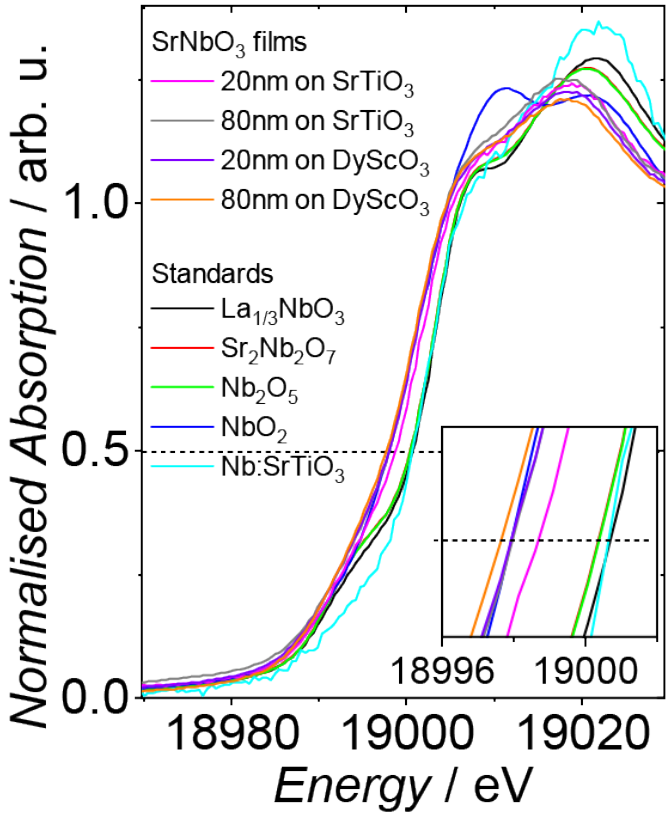


Figure S 14 Normalised absorption edge from XANES experiment of nominally 20nm and 80nm $SrNbO_3$ films on $SrTiO_3$ and $DyScO_3$ substrates and standards

Transmission

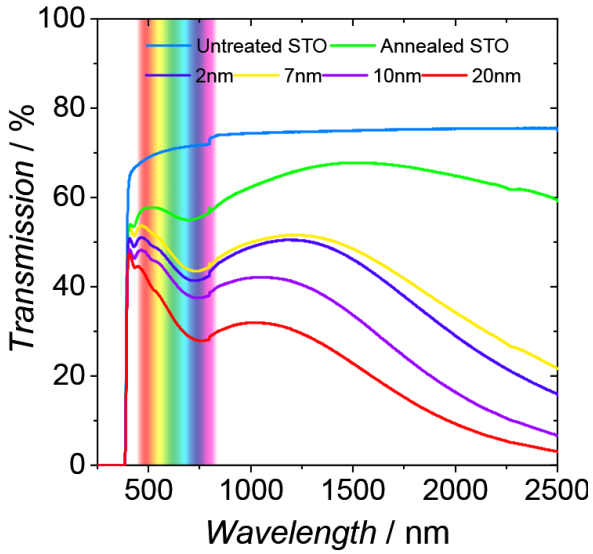


Figure S 15. UV-visible-NIR transmission spectra of SNO films of different thickness on double polished STO substrates. Colour section corresponds to visible region of the spectrum.

Transport Data

Table S1: Electrical transport data for a series of thickness of $SrNbO_3$ films on $SrTiO_3$, $DyScO_3$ and LSAT substrates

Substrate	$SrNbO_3$ Film Thickness (nm)	ρ(300K) (μΩcm)	ρ(2K) (μΩcm)	RRR	μ(2K) ($cm^2V^{-1}s^{-1}$)	n(2K) ($x10^{22}cm^{-3}$)
$SrTiO_3$ (0 0 1)	2	6.1	0.003	2015	47290	4.36
	5	4.4	0.002	2082	52700	5.62
	7	5.0	0.002	3123	-	-
	19	9.7	0.007	1463	41330	2.26
	39	12.8	0.009	1430	38290	1.82
	61	12.6	0.012	1012	32350	1.55
	74	11.3	0.008	1381	43400	1.75
$SrTiO_3$ (1 1 1)	23	14.6	0.007	2142	48340	2.01
LSAT (0 0 1)	16	69.8	61.7	1.13	11.3	0.89
$DyScO_3$ (1 1 0)	70	48.9	43.0	1.38	*	*

*The Hall resistance could not be measured due to the paramagnetic nature of $DyScO_3$.

Substrate treatment was minimal, with cleaning in ethanol and drying with N_2. No chemical etching was done.

The resistivity is calculated from the thickness observed from the XRR

TCM Properties

Samples deposited on double-side polished $SrTiO_3$ were used for UV-Vis transmission measurements and the room temperature resistance measured.

Table S 2: TCM properties and FOM values for $SrNbO_3$ + charge transfer systems with varying film thickness. Average transmission determined from Ellipsometry.

$SrNbO_3$ Film Thickness (nm)	R_s (Ω/□)	Average Transmission (400 – 800 nm)	FOM ($\times 10^{-2}\ \Omega^{-1}$)
2	30.5	0.76	0.211
5	8.8	0.44	0.00309
17	6.2	0.83	4.25
19	5.1	0.82	2.69
39	3.3	0.67	0.555
61	2.1	0.55	0.123
74	1.5	0.48	0.0425