Supporting Information (SI)

On the thermoelectric properties of Nb-doped $SrTiO_3$ epitaxial thin films

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I: Calculation of out-of-plane lattice constants by using Poisson ratio

Calculation of the expected *c*-parameter of film from Poisson ratio (ν) is obtained by using the following relations:

$$\nu = -\frac{\epsilon_t}{\epsilon_l}$$

$$\epsilon_t = \frac{(out-of-plane,\ c)_{film} - c_{bulk}}{c_{bulk}}$$

$$\epsilon_l = \frac{(in-plane,\ a)_{film} - a_{bulk}}{a_{bulk}}$$

Assuming a material is stretched or contracted in axial direction against in-plane compressive or tensile strain, then ν is given by the ratio of transverse strain (ϵ_t) to axial strain (ϵ_l)[1]. In our case, films are epitaxial and compressively strained (-1.33%) on LSAT substrates. Hence, the in-plane (a_{film}) parameters of the films are same as LSAT substrates (LSAT, a = 3.870 Å) and the a-parameter of bulk $SrTi_{0.94}Nb_{0.06}O_3$ is known, $a_{bulk} = 3.922$ Å (see main text[2]). Hence, ϵ_l can be calculated. On the other hand, $\nu = 0.23$ is known for standard perovskites (see main text[3]) and c_{bulk} is known for $SrTi_{0.94}Nb_{0.06}O_3$. Therefore, theoretical c_{film} value can be calculated considering an elastic strain.

II: Additional tables

Table S1 Calculated parameters obtained from DFT-based calculations by using a fixed in-plane (3.870 Å) and variable out-of-plane (3.870, 3.906, 3.970 and 3.980 Å) lattice constants of Nb:STO bulk structure.

c-parameter (Å)	η-chemical potential (eV)	*n* (×10^{21}, cm^{-3})	Effective mas $m_e(m_0)$ G-Z	Effective mas $m_h(m_0)$ G-M	Ti-d orbital position
3.870	-1.146	2.057	0.709 (G-M)	-2.626	$d_{xy}=d_{xz}=d_{yz}$ (at gamma point), Δd=0 eV
3.906	-1.140	2.104	0.318	-0.756	$d_{xy}>d_{xz}=d_{yz}$ (at gamma point), Δd=0.0122 eV
3.970	-1.121	2.019	0.337	-0.784	$d_{xy}>d_{xz}=d_{yz}$ (at gamma point), Δd=0.0377 eV
3.980	-1.117	2.056	0.339	-0.782	$d_{xy}>d_{xz}=d_{yz}$ (at gamma point), Δd=0.0432 eV

Table S2 *calculated chemical potential (η) and Seebeck coefficients (S) at 290K from the measured density of charge carriers (n) by using equation (1-4) in the main text for 31 and 11 nm thick Nb:STO films at variable electron band degeneracy (z) and scattering parameter (r). calculations are done by assuming a fixed effective mass of electrons m* (=1.1m_0, where m_0 is the rest mass of electrons).*

Thickness (nm)	n (cm^{-3})	$\|\eta\|$ (ev)		S (μV/K) for z=6			S (μV/K) for z=4		
		z=6	z=4	r=1	r=1.5	r=2	r=1	r=1.5	r=2
32	1.7×10^{21}	0.28	0.30	-59	-73	-87	-46	-57	-68
11	9.5×10^{20}	0.15	0.20	-86	-105	-124	-67	-83	-98

Table S3 Lattice parameters, and calculated band gap of 6%Nb-doped $SrTiO_3$ at the SCAN meta-GGA level.

Lattice parameter (Å)	3.87	3.906	3.97	3.98
Band gap (eV)	1.806	1.797	1.735	1.728

III: Additional figures

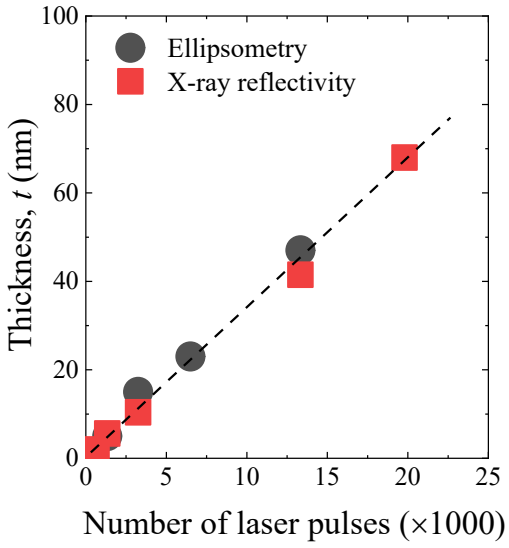

Fig. S1. *Thickness measurements of the Nb:STO films on LSAT substrates by using x-ray reflectivity and ellipsometry techniques.*

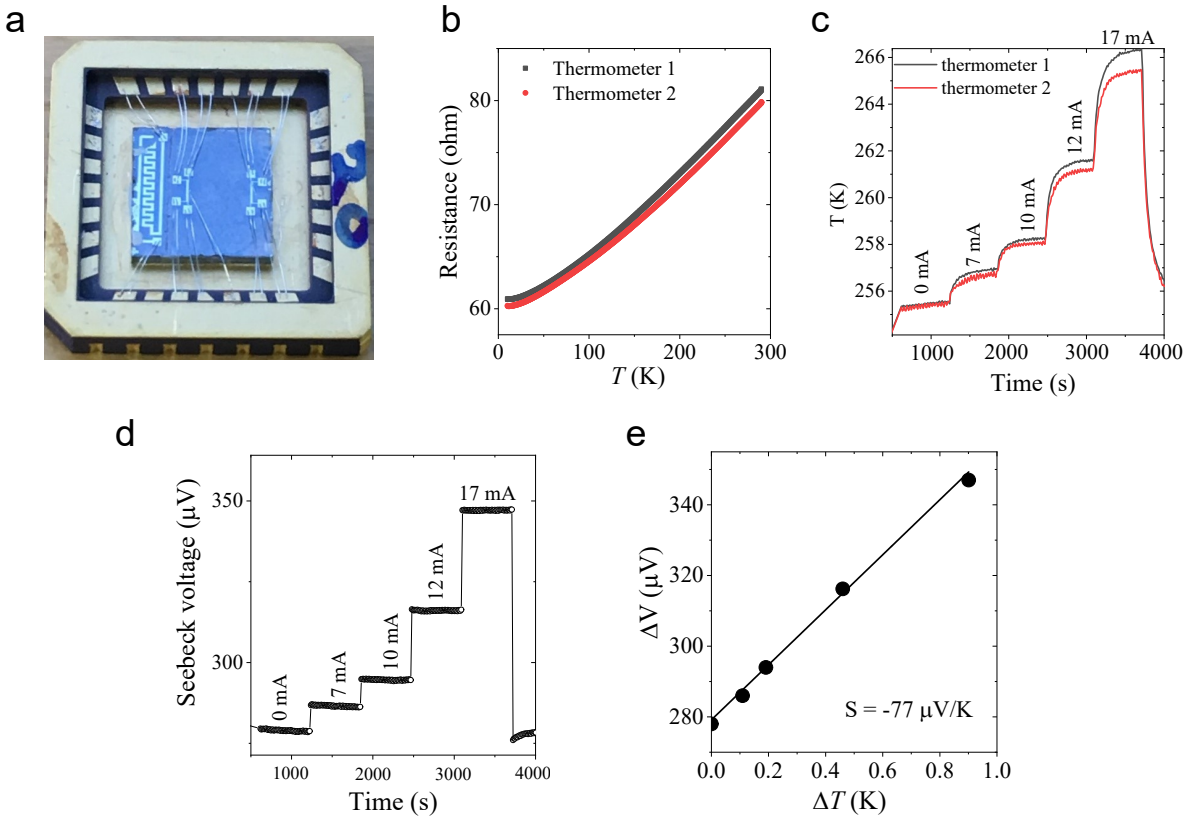

Fig. S2. *Schematic illustration of the Seebeck effect measurement on Nb:STO thin films. A Pt heater and two Pt-resistors/thermometers were patterned on top of the film surface by using optical lithography techniques. a- An actual image of the wire-boned Nb:STO film prepared on a chip-carrier for Seebeck coefficient measurement. b- Resistance calibration of the two Pt-resistors as a function of temperature. These files were later used to define temperature difference. c- Real time temperature measurement of the two-resistors when a variable current applied to the Pt heater and, d- at the same time Seebeck voltage measurements. e- Seebeck coefficients were calculated from the slope of the ΔV vs ΔT curve.*

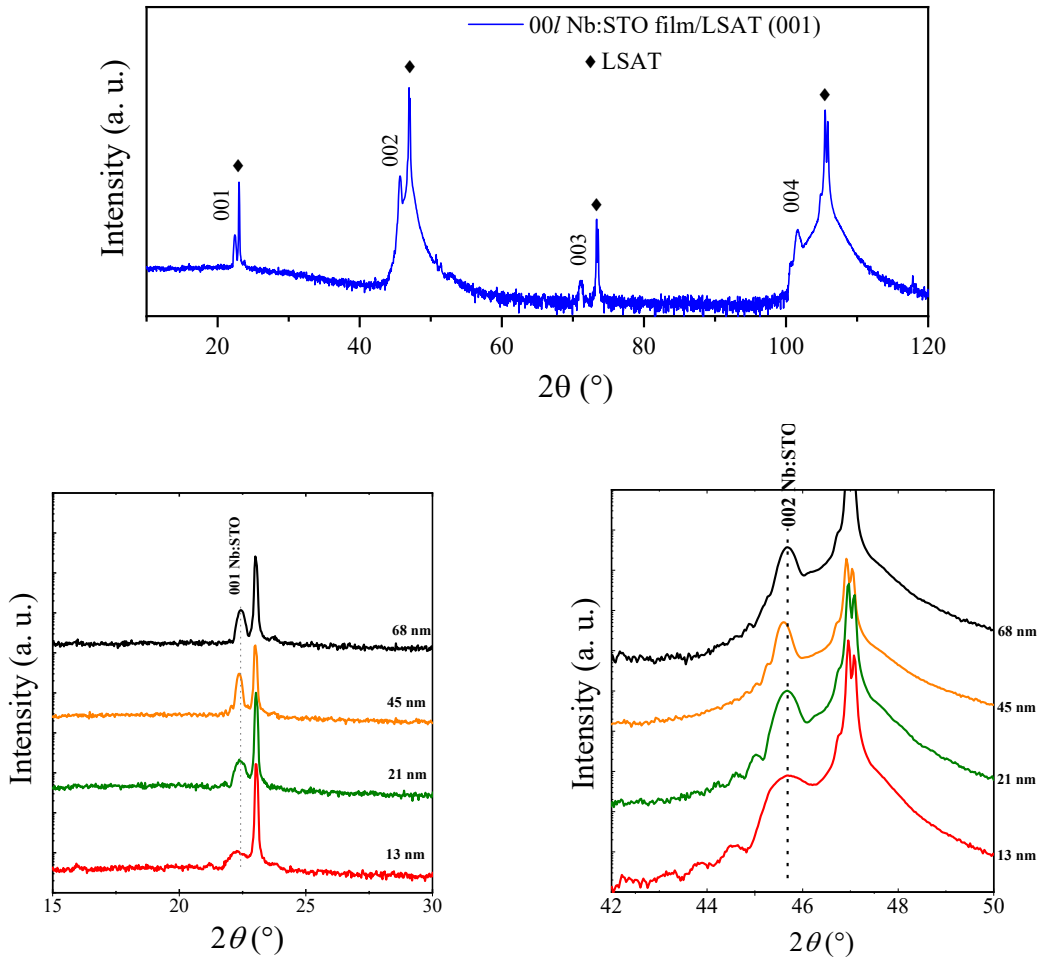

Fig. S3. *X-ray diffraction patterns of Nb:STO films deposited on LSAT-001 substrates.*

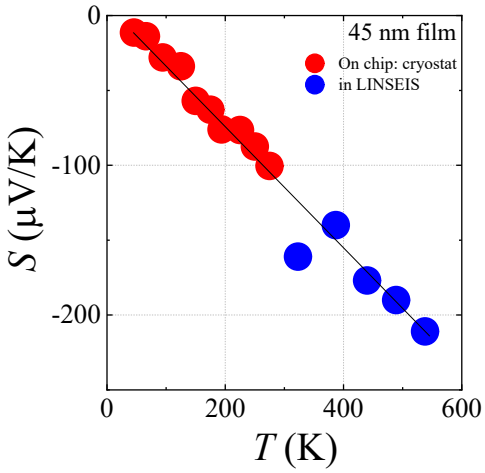

Fig. S4. *Seebeck coefficient measurements of Nb:STO films by two different techniques over a long range of temperature: on-chip Seebeck measurement in a cryostat between 20-300 K and in a LINSEIS instrument within 300-550 K.*

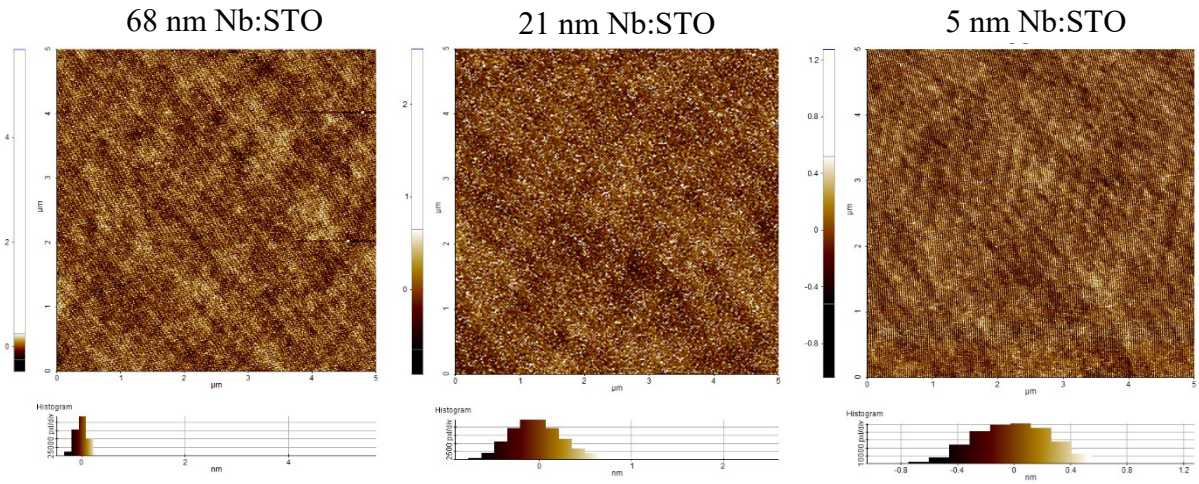

Fig. S5. AFM-topography images of Nb-doped $SrTiO_3$ films on LSAT substrates.

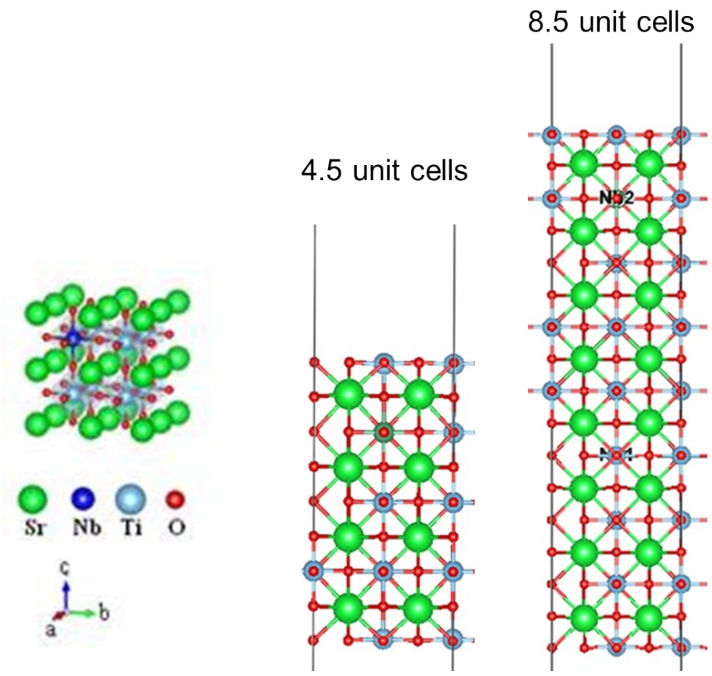

Fig. S6. Bulk crystal structures of Nb-doped $SrTiO_3$, and unit cells of Nb-doped $SrTiO_3$ films were considered for electronic band structure calculations.

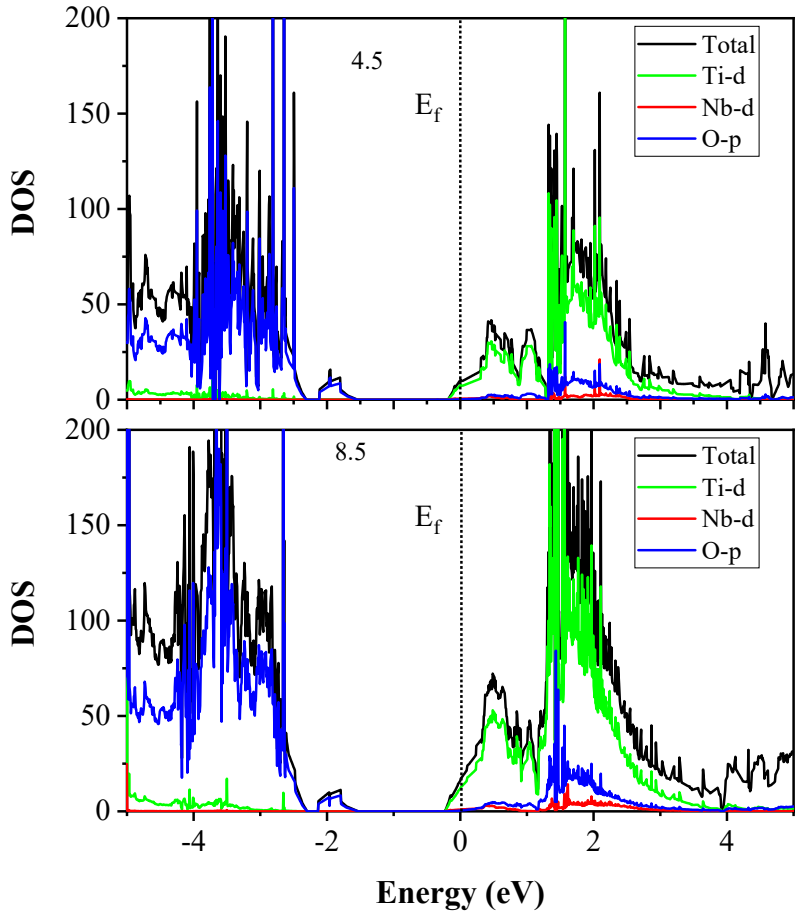

Fig. S7. Calculated electronic band structures for 4.5, and 8.5 unit cells thick Nb-doped $SrTiO_3$ films.

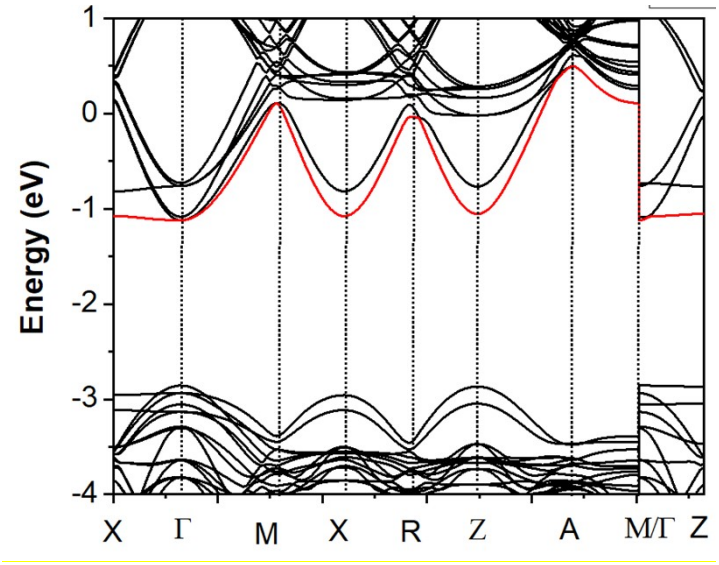

Fig. S8 The effective mass calculation by fitting a quadratic function ($y=A+Bx+Cx^2$) at the band edge from the first conduction band as highlighted by the red-line.

References

[1] L. Iglesias, A. Sarantopoulos, C. Magén, and F. Rivadulla, Phys. Rev. B **95**, 165138 (2017).

[2] B. Zhang, J. Wang, T. Zou, S. Zhang, X. Yaer, N. Ding, C. Liu, L. Miao, Y. Li, and Y. Wu, J. Mater. Chem. C **3**, 11406 (2015).

[3] H. Ledbetter, M. Lei, and S. Kim, Phase Transitions **23**, 61 (1990).