Supporting Information

Influence of redox engineering on the trade-off relationship between thermopower and electrical conductivity in lanthanum titanium based transition metal oxides

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Weighted carrier properties calculation

The weighted mobility (μ_w) is a measure of the electron mobility weighted by the density of electronic states.[1] The weighted mobility, like the hall mobility, can be defined as a simple function of two measured properties, S and σ.[1] The following equation is a simple analytic form for μ_w:[1]

$$\mu_w = \frac{3h^3\sigma}{8\pi e(2m_e k_B T)^{3/2}}\left[\frac{exp\left(\frac{|S|}{k_B/e} - 2\right)}{1 + exp\left(-5\left(\frac{|S|}{k_B/e} - 1\right)\right)} + \frac{\frac{3}{\pi^2}\frac{|S|}{k_B/e}}{1 + exp\left(5\left(\frac{|S|}{k_B/e} - 1\right)\right)}\right]$$

Where h is Planck's constant (eV · s), σ is the electrical conductivity (S/cm), e is the electron charge (eV), k_B the Boltzmann constant (eV/K), T is the operating temperature, and S is the thermopower (μV/K).

The weighted carrier properties can be obtained using the calculated μ_w. The weighted carrier concentration (n_w) was calculated using the formula below:[2]

$$n_w = \frac{\sigma}{\mu_w e}$$

The relaxation time (τ_w) was obtained by using the following equation:[3]

$$\tau_w = \frac{m_w^* \mu_w}{e}$$

Where m^*_w is the weighted effective mass which was calculated by using the following equation: [4]

$$\frac{m_w^*}{m_e} = \frac{3eh^2 \times S}{8\pi^2 k_B^2 \times T \times (\pi/3n_w)^{2/3}}$$

Where m_e is the mass of an electron.

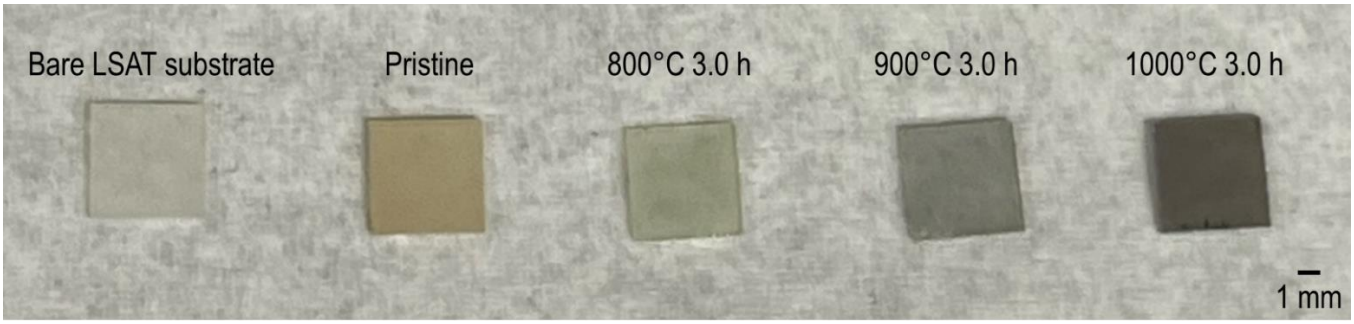

Fig. S1: Picture of the bare LSAT substrate and LCNTO thin films grown on LSAT substrates exposed to different reduction conditions.

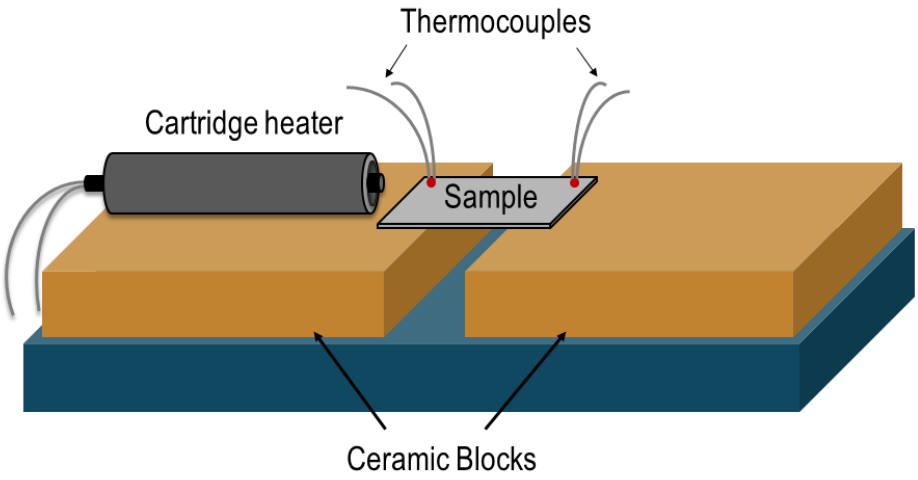

Fig. S2: Schematic of the measurement setup that was used to measure *S*.

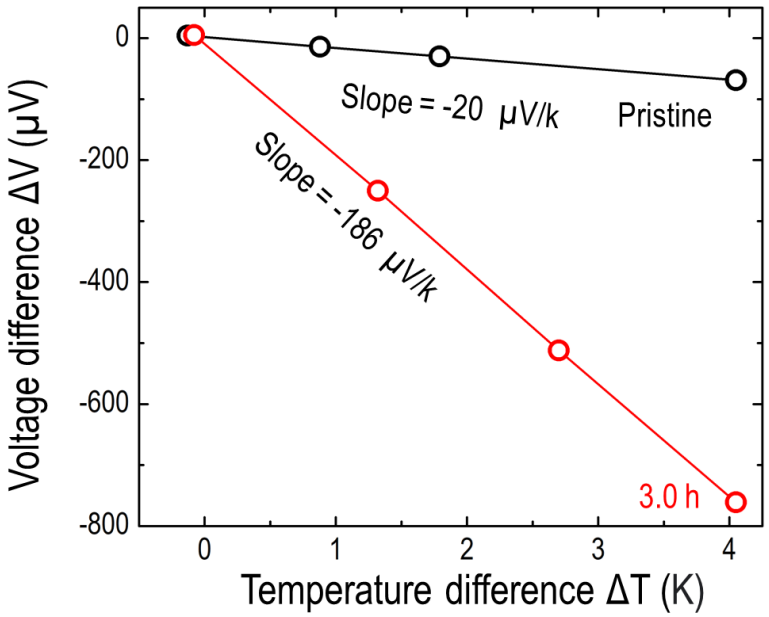

Fig. S3: Voltage difference (ΔV) as a function of Temperature difference (ΔT) measured at room temperature with the pristine and reduced LCNTO films at 900°C for 3.0 h. *S* was extracted from the different slopes (ΔV/ΔT) of both samples.

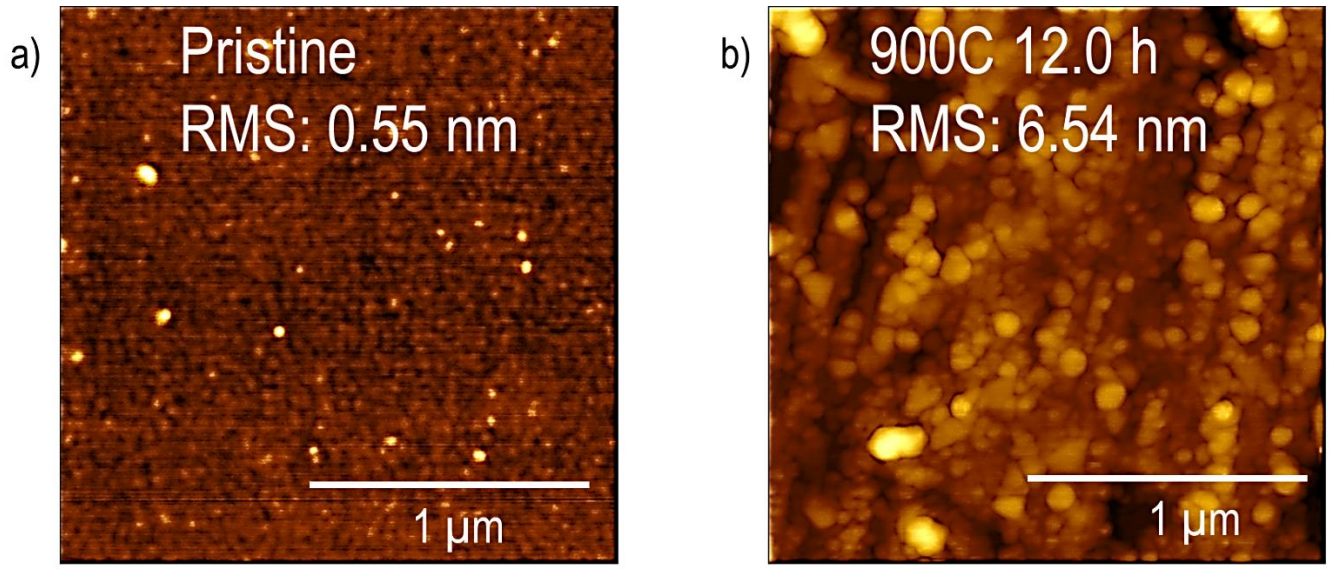

Fig. S4: AFM images of the (a) pristine LCNTO film and (b) LCNTO film reduced at 900°C for 12.0 h.

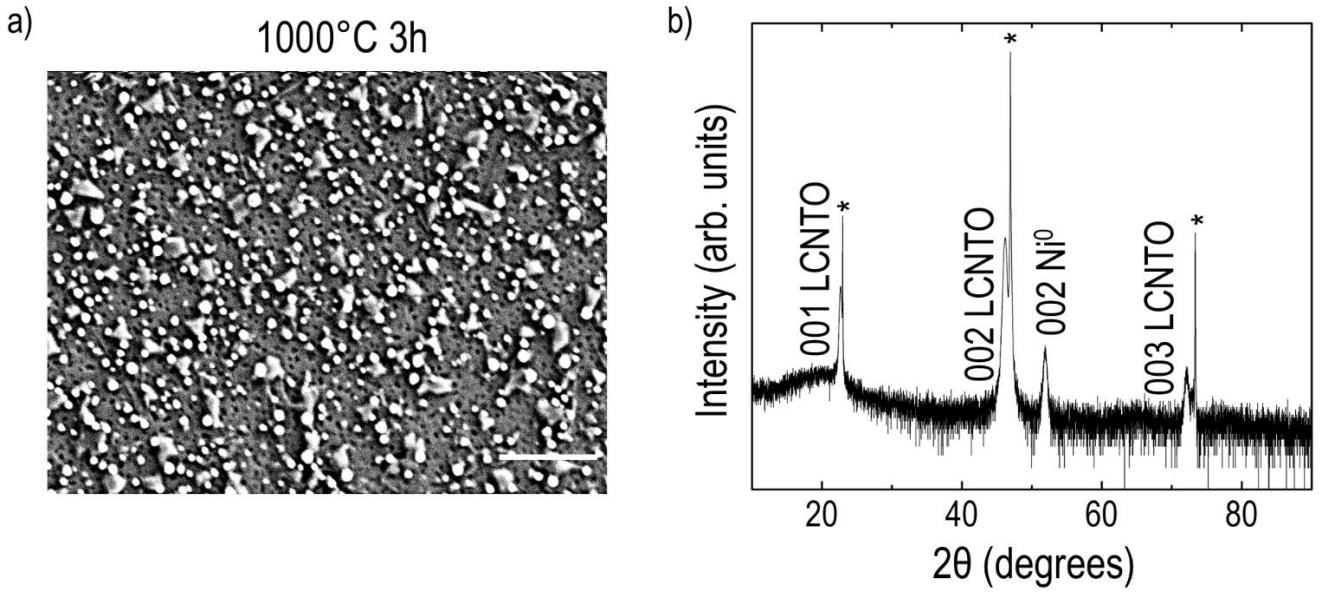

Fig. S5: (a) SEM images of the surface of LCNTO thin films reduced under 1000 °C for 3.0 h (scale bar: 1 μm). (b) XRD θ-2θ patterns of the reduced LCNTO thin films at 1000°C for 3.0 h (Substrate peaks are indicated with *).

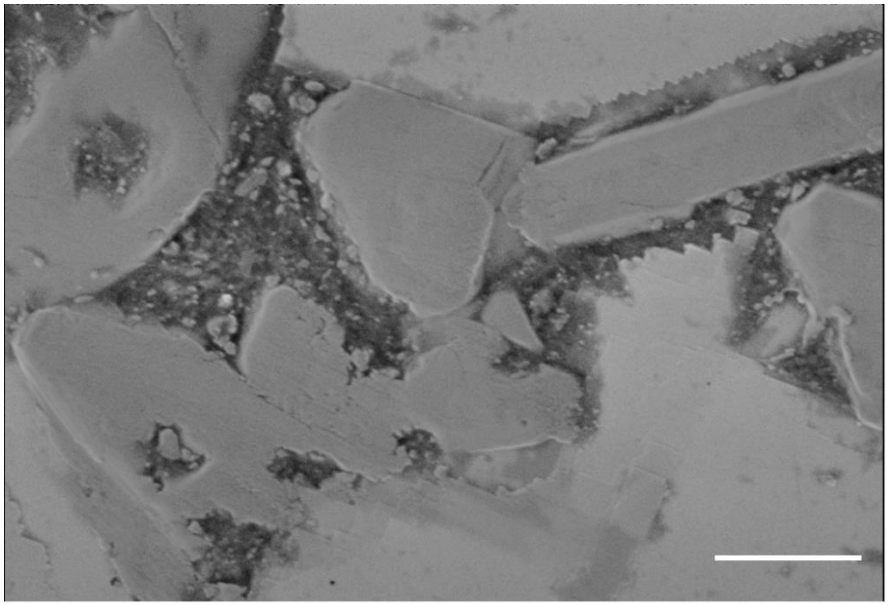

Fig. S6: SEM image of the surface of LCNTO thin films post-annealed in air under 1200 °C for 12.0 h (scale bar: 1 μm).

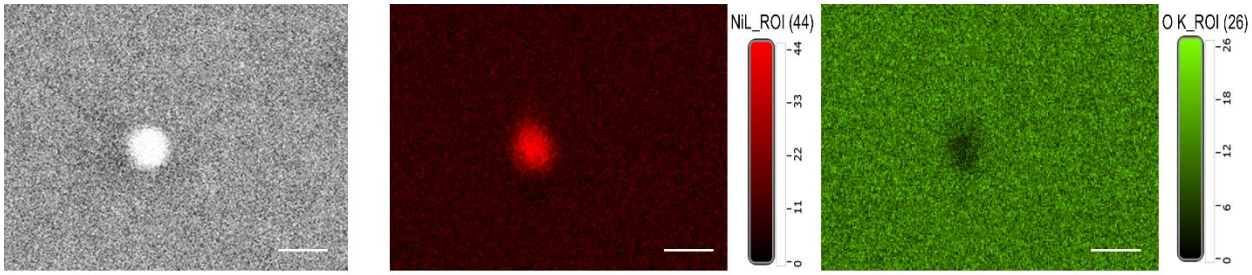

Fig. S7. Top view SEM image of LCNTO film reduced at 900°C for 3.0 h and its corresponding Nickel and Oxygen EDX map (scale bar: 100 nm).

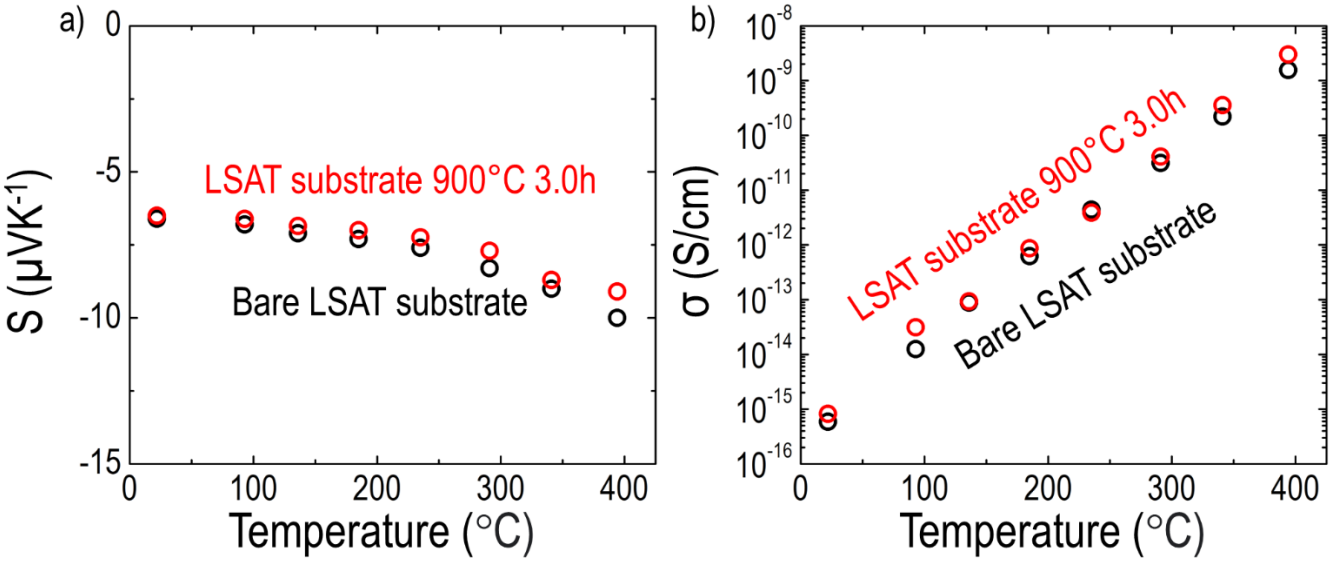

Fig. S8: Temperature dependencies of (a) *S* and (b) σ of the pristine LSAT substrate (black) and reduced LSAT substrate at 900°C for 3.0 h (red) measured from 20 to 400°C.

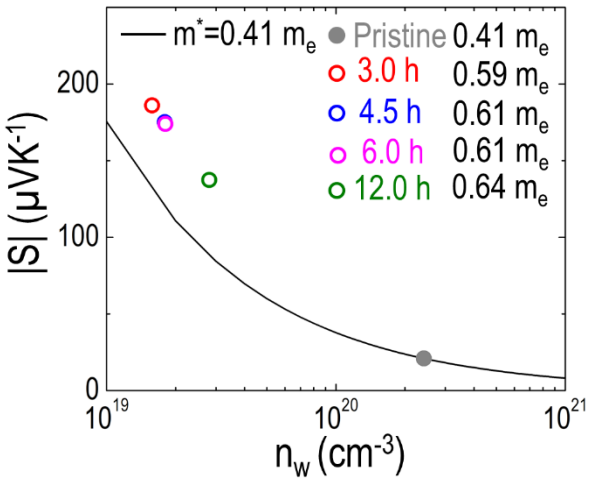

Fig. S9. Pisarenko relation (variation of |S| with n_w) for the LCNTO thin films before and after reduction at 900 °C with varying reduction time at room temperature.

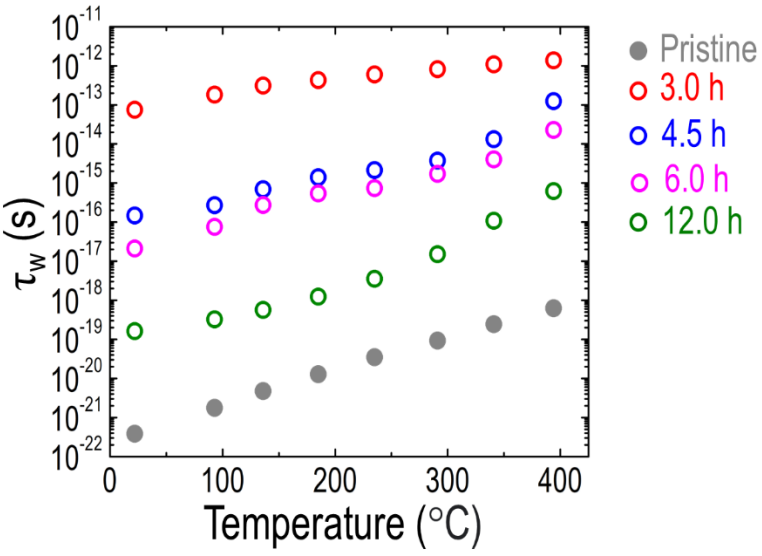

Fig. S10: Temperature dependencies of τ_w of the pristine and reduced LCNTO thin films at 900 °C with varying reduction time.

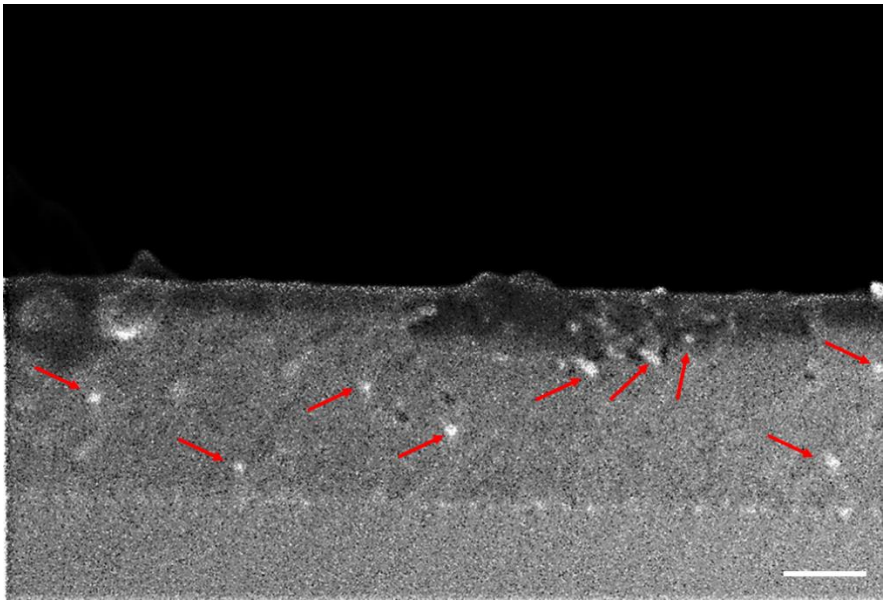

Fig. S11. Cross-sectional SEM image of LCNTO film reduced at 900°C for 12.0 h. The red arrows indicate Ni particles (scale bar: 100 nm).

References

1. G. J. Snyder, A. H. Snyder, M. Wood, R. Gurunathan, B. H. Snyder and C. Niu, *Advanced Materials*, 2020, **32**, 2001537.
2. T. Katase, X. He, T. Tadano, J. M. Tomczak, T. Onozato, K. Ide, B. Feng, T. Tohei, H. Hiramatsu and H. Ohta, *Advanced Science*, 2021, **8**, 2102097.
3. M. Massetti, F. Jiao, A. J. Ferguson, D. Zhao, K. Wijeratne, A. Würger, J. L. Blackburn, X. Crispin and S. Fabiano, *Chemical Reviews*, 2021, **121**, 12465-12547.
4. X. Zhang and L.-D. Zhao, *Journal of Materiomics*, 2015, **1**, 92-105.