

High-throughput Parasitic-independent Probe Thermal Resistance Calibration for Robust Thermal Mapping with Scanning Thermal Microscopy

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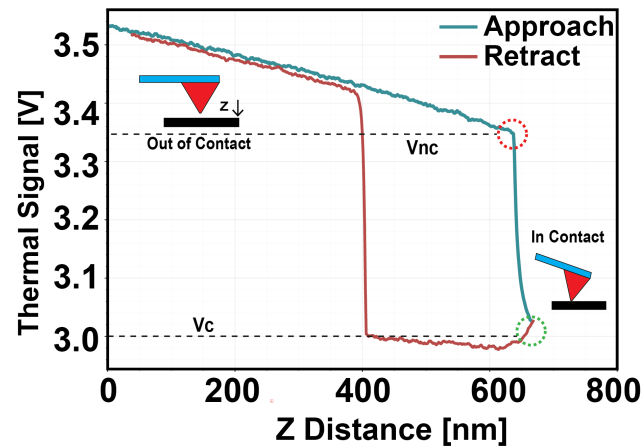


Figure S. 1. Thermal signals recorded during the approach–retract cycle of the SThM probe on the sample surface.

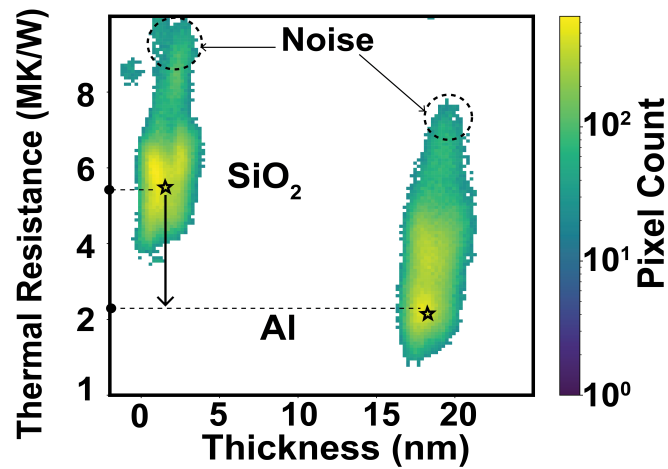


Figure S. 2. 2D histogram of pixel-to-pixel correlation between the height and thermal resistance map.

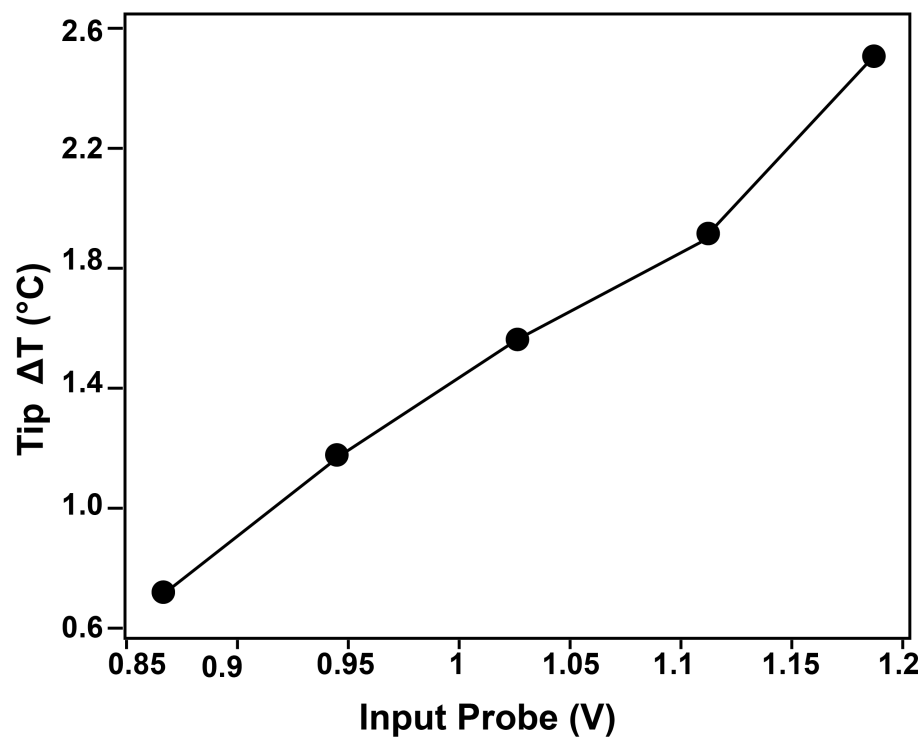


Figure S. 3. Calibration of the thermo-resistive probe for SThM. The resulting change in temperature (ΔT) is calculated from the measured change in resistance (ΔR) using the vendor-provided thermal coefficient of resistance (TCR), α , which is defined as: $\Delta T \approx \frac{1}{R_0 \alpha} \Delta R$ This calibration step establishes the critical relationship between the electrical signal (voltage/resistance) and the temperature of the probe tip, which is essential for converting raw SThM data into a quantitative thermal map.

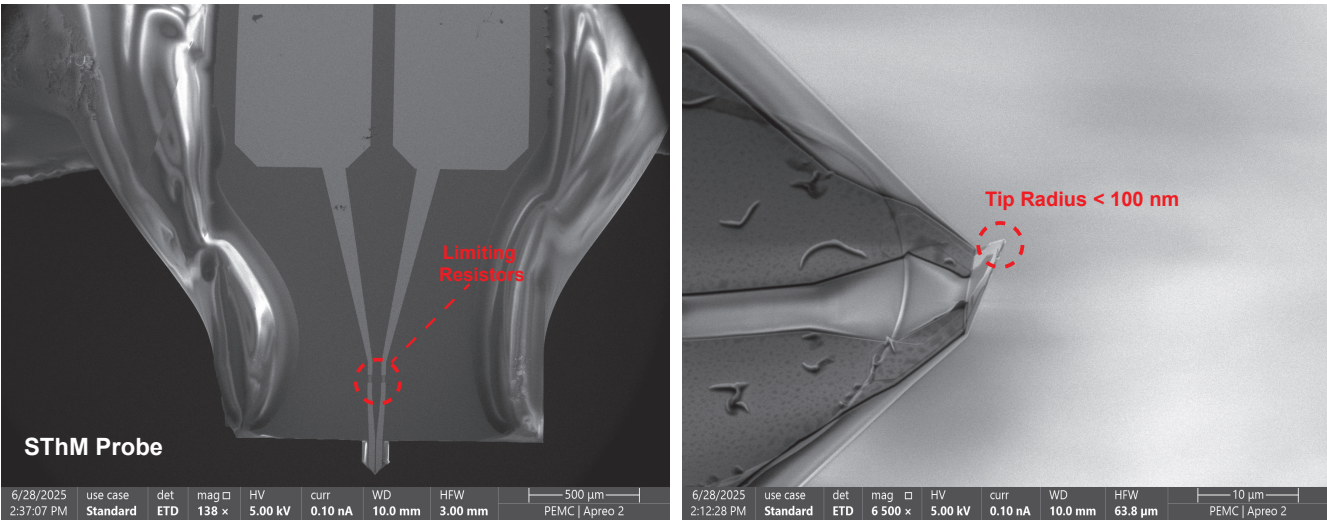


Figure S. 4. SEM images of the SThM probe.

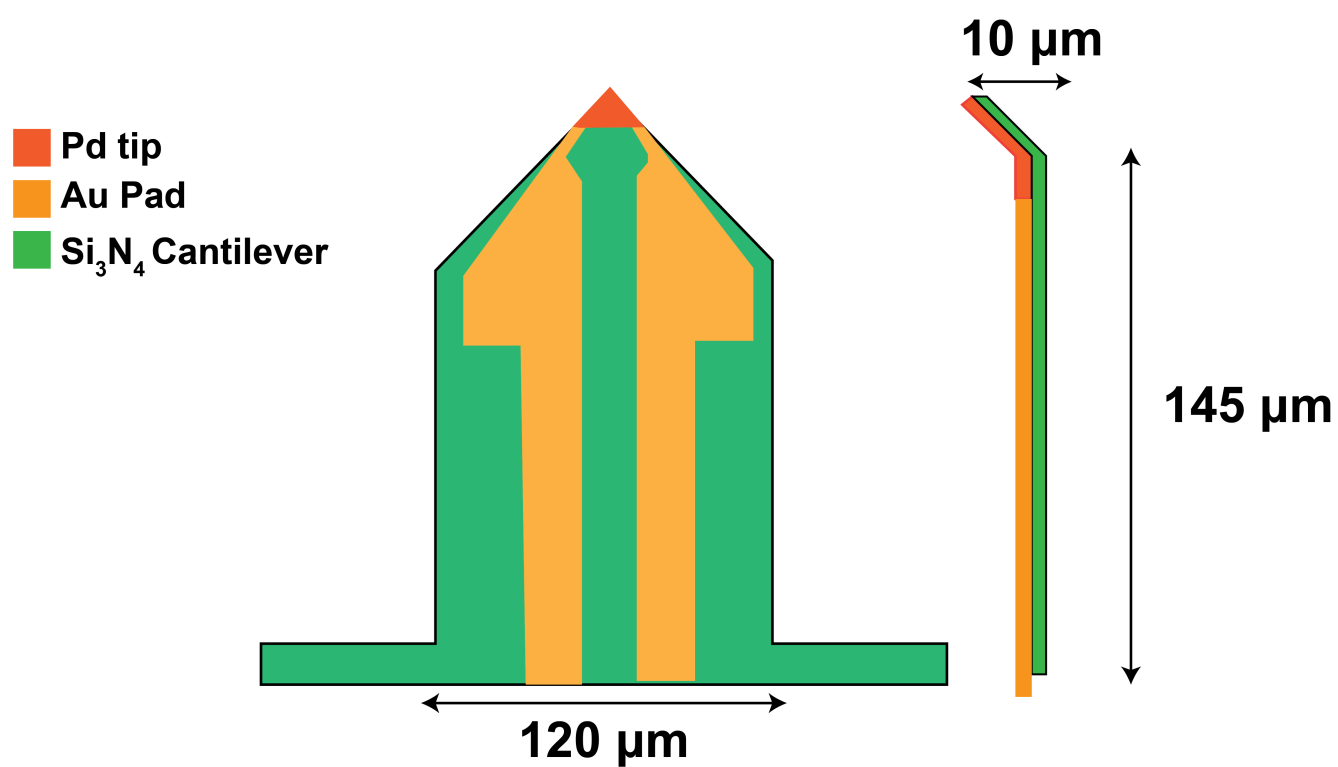


Figure S. 5. Geometry of the SThM probe used in this study.

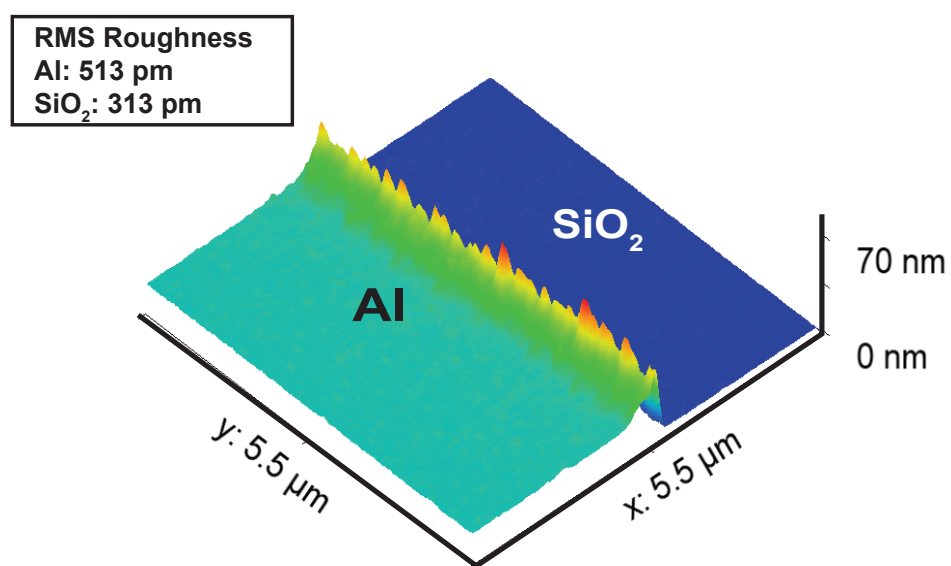


Figure S. 6. 3D AFM topography map of the Al/SiO₂ surface, indicating uniform morphology with comparable roughness, thereby minimizing topography-induced artifacts in subsequent SThM measurements.

TABLE S. I. Experimental parameters for the Al/SiO₂/Si system.

Parameter	Value	Source
Tip contact radius, b	50 nm	SEM
Al film thickness, t	14 ± 1 nm	AFM
SiO ₂ thickness	1500 nm	Manufacturer
k_{SiO_2}	1.38 W/(m·K)	Ref.1
k_{Si}	150 W/(m·K)	Refs.2 and 3
h_{BD} (Al/SiO ₂)	150–250 MW/(m ² K)	Refs.2 and 3
R_{meas} (Al sample)	2.60 MK/W	Experiment
R_{meas} (SiO ₂ reference)	5.41 MK/W	Experiment

S1. PIXEL DWELL TIME AND SAMPLE THERMAL DIFFUSION TIME

The AFM scan rate f is defined as the number of scan lines acquired per second. Accordingly, the time required to acquire a single scan line is given by

$$t_{\text{line}} = \frac{1}{f}. \quad (\text{S1.1})$$

For an image consisting of N pixels per line, the corresponding pixel dwell time is

$$t_{\text{pixel}} = \frac{t_{\text{line}}}{N} = \frac{1}{fN}. \quad (\text{S1.2})$$

For scan rates in the range $f = 0.5\text{--}1$ Hz and image sizes of $N = 256$ and 512 pixels per line, the pixel dwell time spans the following ranges:

$$t_{\text{pixel}}^{256} = \frac{1}{f \times 256} = 3.9\text{--}7.8 \text{ ms}, \quad (\text{S1.3})$$

$$t_{\text{pixel}}^{512} = \frac{1}{f \times 512} = 1.95\text{--}3.9 \text{ ms}. \quad (\text{S1.4})$$

For typical SThM conditions, the characteristic thermal interaction length scale is on the order of $L \sim 50\text{--}100$ nm. Using representative thermal diffusivities of $\alpha \sim 10^{-4}$ m²/s for metals (e.g., Al, Au) and $\alpha \sim 10^{-6}$ m²/s for insulating oxides (e.g., SiO₂), the corresponding sample diffusion times are

$$\tau_s^{\text{metal}} \sim 10^{-11}\text{--}10^{-10} \text{ s}, \quad \tau_s^{\text{insulator}} \sim 10^{-9}\text{--}10^{-8} \text{ s}. \quad (\text{S1.5})$$

These times are several orders of magnitude shorter than the millisecond-scale pixel dwell times employed in this work, indicating that the sample temperature field equilibrates quasi-instantaneously during scanning.

S2. ITERATIVE SOLUTION ALGORITHM

Algorithm 1 Iterative Thermal Conductivity Extraction

Require: $h_{\text{BD}}, t, b, k_{\text{sub}}, R_{\text{meas}}, R_{\text{int}}, \text{tolerance } \varepsilon$

Ensure: $k_{\text{film}}, f, L_{\text{spread}}$

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1:  $R_{\text{avail}} \leftarrow R_{\text{meas}} - R_{\text{int}}$                                 ▷ Available resistance for spreading + interface
2:  $R_{\text{BD,contact}} \leftarrow 1/(h_{\text{BD}} \cdot \pi b^2)$                     ▷ Contact interface resistance
3: Initial guess: Solve  $R_{\text{spr}}(k^{(0)}) = R_{\text{avail}}$                 ▷ Ignoring interface
4: for  $n = 1, 2, \dots, N_{\text{max}}$  do
5:    $L^{(n)} \leftarrow t \cdot \sqrt{k^{(n-1)}/k_{\text{sub}}}$                 ▷ Update spreading length
6:    $f^{(n)} \leftarrow (b/(b + L^{(n)}))^2$                         ▷ Update dilution factor
7:    $R_{\text{BD,eff}}^{(n)} \leftarrow f^{(n)} \cdot R_{\text{BD,contact}}$           ▷ Effective interface resistance
8:    $R_{\text{spr,target}}^{(n)} \leftarrow R_{\text{avail}} - R_{\text{BD,eff}}^{(n)}$         ▷ Target spreading resistance
9:   Solve  $R_{\text{spr}}(k^{(n)}) = R_{\text{spr,target}}^{(n)}$  for  $k^{(n)}$         ▷ Using Brent's method
10:  if  $|k^{(n)} - k^{(n-1)}|/k^{(n-1)} < \varepsilon$  then
11:    converged
12:    return  $k^{(n)}, f^{(n)}, L^{(n)}$ 
13:  end if
14: end for
15: return not converged

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The algorithm typically converges in 5–15 iterations for $\varepsilon = 10^{-8}$. Convergence is guaranteed because:

1. $R_{\text{spr}}(k)$ is monotonically decreasing in k
2. $f(k)$ is monotonically decreasing in k (larger k means more spreading)
3. The product $f(k) \cdot R_{\text{BD}}$ decreases with increasing k
4. Therefore, the iteration is a contraction mapping

S3. THERMAL CONDUCTIVITY AND UNCERTAINTY CALCULATION FOR 15 NM ALUMINUM THIN FILM

A. Reference Measurement

1. Tip Interface Resistance Extraction

Step 1: Calculate $R_{\text{spr}}(\text{SiO}_2/\text{Si})$ using Equation 14

Using $k_{\text{SiO}_2} = 1.38 \text{ W}/(\text{m}\cdot\text{K})$, $k_{\text{Si}} = 150 \text{ W}/(\text{m}\cdot\text{K})$, $t = 1500 \text{ nm}$, $b = 50 \text{ nm}$:

$$R_{\text{spr}}(\text{SiO}_2/\text{Si}) = 3.57 \text{ MK/W}$$

Step 2: Extract tip interface resistance

$$R_{\text{int}}(\text{tip}) = R_{\text{meas}}(\text{SiO}_2) - R_{\text{spr}}(\text{SiO}_2/\text{Si}) = 5.41 - 3.57 = 1.84 \text{ MK/W}$$

This interface resistance is assumed constant for both SiO_2 and Al surfaces, as both measurements use the same tip and similar contact mechanics.

TABLE S. II. Extracted k_{Al} (W/(m·K)) for different h_{BD} and thickness combinations.

h_{BD} (MW/(m ² K))	$t = 13$ nm	$t = 14$ nm	$t = 15$ nm
150	52.1	48.0	44.5
175	50.2	46.3	43.0
200	48.8	45.1	41.9
225	47.8	44.2	41.1
250	46.9	43.4	40.4

B. Iterative Algorithm for k Extraction

1. The Self-Consistency Problem

Both R_{spr} and the dilution factor f depend on k_{Al} , which is the unknown:

$$R_{spr} = R_{spr}(k_{Al}) \quad (\text{Yovanovich integral}) \quad (S3.1)$$

$$f = f(k_{Al}) = \left[\frac{b}{b + t \sqrt{k_{Al}/k_{SiO_2}}} \right]^2 \quad (S3.2)$$

This requires an iterative solution.

Algorithm:

1. Calculate available resistance: $R_{avail} = R_{meas}(Al) - R_{int} = 2.60 - 1.84 = 0.76$ MK/W
2. Initial guess: Solve $R_{spr}(k^{(0)}) = R_{avail}$ (ignoring interface)
3. Iterate until convergence:
 - (a) Compute $L^{(n)} = t \cdot \sqrt{k^{(n-1)}/k_{SiO_2}}$
 - (b) Compute $f^{(n)} = [b/(b + L^{(n)})]^2$
 - (c) Compute $R_{BD,eff}^{(n)} = f^{(n)}/(h_{BD} \cdot \pi b^2)$
 - (d) Solve $R_{spr}(k^{(n)}) = R_{avail} - R_{BD,eff}^{(n)}$
 - (e) Check: if $|k^{(n)} - k^{(n-1)}|/k^{(n-1)} < 10^{-8}$, stop

Convergence: At $h_{BD} = 200$ MW/(m²K), $t = 14$ nm:

$$k_{Al} = 45.1 \text{ W/(m} \cdot \text{K)} \quad (10 \text{ iterations})$$

S4. S4. THEORETICAL THERMAL CONDUCTIVITY PREDICTION

A. S4.1 Combined Fuchs-Sondheimer and Mayadas-Shatzkes Model

The thermal conductivity of metallic thin films is reduced from bulk values due to electron scattering at surfaces and grain boundaries. The combined model is:

$$k_{film} = k_{e,bulk} \times f_{FS} \times f_{MS} + k_{ph} \quad (S4.1)$$

where $k_{e,bulk} = 231$ W/(m·K) is the bulk electronic thermal conductivity, $k_{ph} = 6$ W/(m·K) is the phonon contribution, and f_{FS} , f_{MS} are reduction factors for surface and grain boundary scattering, respectively.

The Fuchs-Sondheimer factor for diffuse surface scattering ($p = 0$) is^{4,5}:

$$f_{FS} = 1 - \frac{3}{2\kappa} \int_0^1 (u - u^3)(1 - e^{-\kappa/u}) du \quad (S4.2)$$

where $\kappa = t/\lambda_e$ is the ratio of film thickness to electron mean free path.

The Mayadas-Shatzkes factor for grain boundary scattering is⁶:

$$f_{\text{MS}} = 3 \left[\frac{1}{3} - \frac{\alpha}{2} + \alpha^2 - \alpha^3 \ln \left(1 + \frac{1}{\alpha} \right) \right] \quad (\text{S4.3})$$

where $\alpha = (\lambda_e/d) \times R/(1-R)$, with d being the grain size and R the grain boundary reflection coefficient.

B. S4.2 Calculation for 14 nm Al Film

Using the literature value $\lambda_e = 19$ nm for aluminum at room temperature⁷, with $d = t = 14$ nm (reasonable approximation for ultra-thin film) and $R = 0.55$ (usual range for polycrystalline film is 0.4 to 0.8):

Step 1: Dimensionless parameters

$$\kappa = \frac{t}{\lambda_e} = \frac{14}{19} = 0.737 \quad (\text{S4.4})$$

$$\alpha = \frac{\lambda_e}{d} \times \frac{R}{1-R} = \frac{19}{14} \times \frac{0.55}{0.45} = 1.659 \quad (\text{S4.5})$$

Step 2: Reduction factors

$$f_{\text{FS}} = 0.614 \quad (\text{numerical integration}) \quad (\text{S4.6})$$

$$f_{\text{MS}} = 3 [0.333 - 0.829 + 2.751 - 2.153] = 0.307 \quad (\text{S4.7})$$

Step 3: Thermal conductivity

$$\begin{aligned} k_{\text{film}} &= k_{e,\text{bulk}} \times f_{\text{FS}} \times f_{\text{MS}} + k_{\text{ph}} \\ &= 231 \times 0.614 \times 0.307 + 6 \\ &= 43.5 + 6 = 49.5 \text{ W/(m} \cdot \text{K)} \end{aligned} \quad (\text{S4.8})$$

C. S4.3 Comparison with Experiment

TABLE S. III. Comparison of theoretical prediction with SThM measurement.

Method	k [W/(m·K)]
F-S + M-S theory ($\lambda_e = 19$ nm)	49.5
SThM measurement (this work)	$45.1^{+4.7}_{-3.6}$

The theoretical prediction of 49.5 W/(m·K) falls within the experimental uncertainty range of 41.5–49.8 W/(m·K), demonstrating good agreement between the SThM-extracted thermal conductivity and the combined Fuchs-Sondheimer and Mayadas-Shatzkes model using the literature electron mean free path for aluminum⁷.

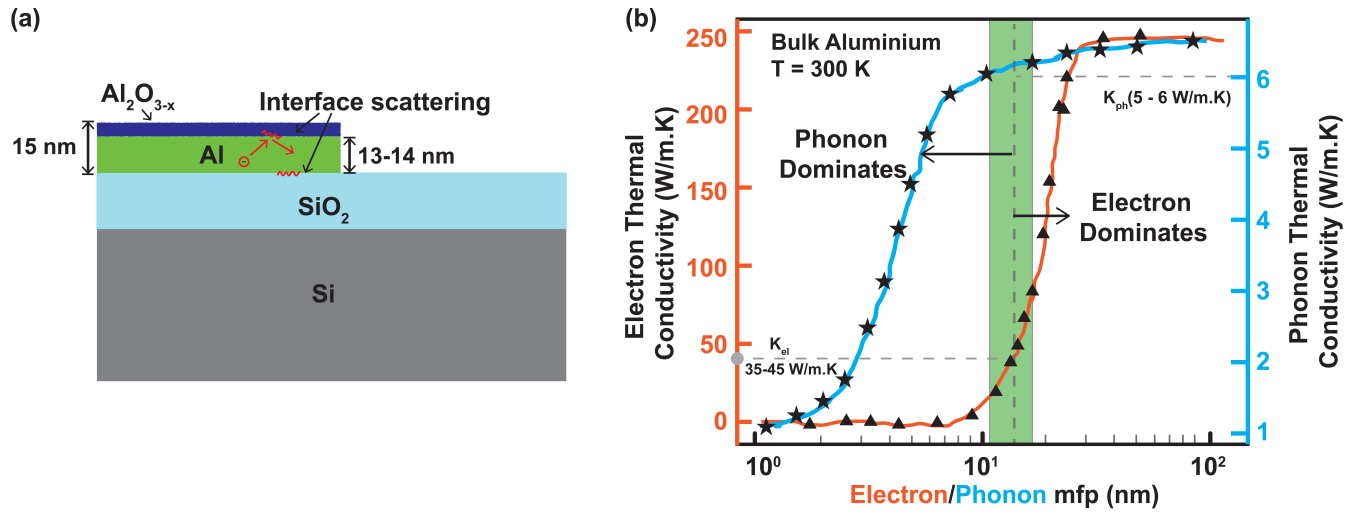


Figure S. 7. (a) Cross-sectional schematic of an Al thin film patterned on a Si/SiO₂ substrate. A native sub-stoichiometric Al₂O_{3-x} layer forms due to exposure to ambient conditions. Interface scattering further reduces the thermal conductivity of both electron and phonon heat carriers. (b) The mean free path (mfp) distributions of both phonon and electron heat carriers in bulk aluminum, derived using their respective thermal conductivity accumulation functions at 300 K. The data in (b) is reproduced from Ref.⁸ with permission from Phys. Rev. B 93, 081206(R). Copyright 2016 American Physical Society.

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