

Supplementary Information:

Photoluminescence, Thermal Transport, and Breakdown in Joule-Heated GaN Nanowires

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Additional high resolution TEM of nanowire featured in Fig. 5.

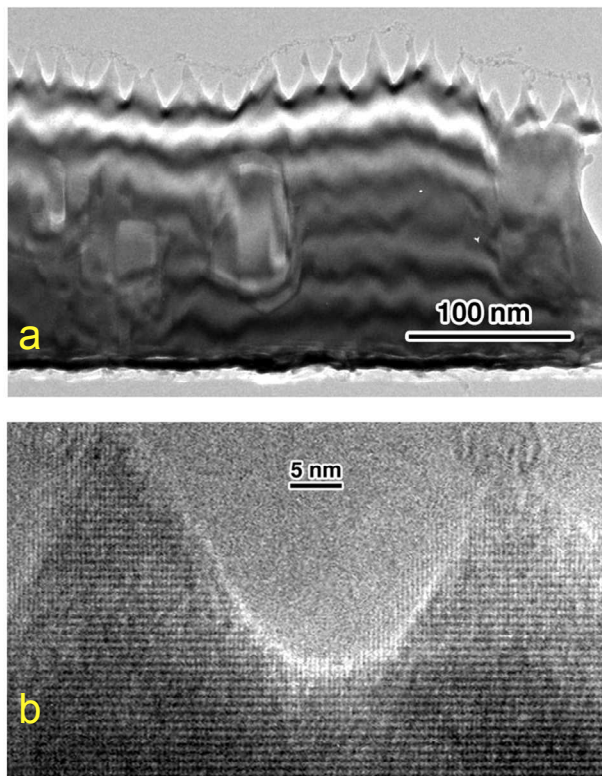


Figure S1. (a) Saw-tooth-like morphology on the surface of the GaN nanowire featured in Fig. 5. (b) High resolution TEM image of one pit on the nanowire surface. The pits are a product of the formation and evaporation of Ga balls at high temperature.

Validity of one-dimensional model

A one-dimensional heat transport model is expedient for fitting experimental data to theory and is justified if two conditions are met. First, the temperature variation within a cross-section of the nanowire must be much less than the temperature rise across the SiO₂ layer (100 nm thick), which behaves as a large thermal resistance between the nanowire and the underlying silicon wafer. The condition specified above is met if the thermal conductivity of the GaN nanowire (50-70 W/m·K) is significantly greater than that of the SiO₂ layer.

The second condition that must be met for a one-dimensional heat transport model to be valid is that heat transport within the SiO₂ layer must occur predominantly in directions perpendicular to the nanowire's axis. This condition is satisfied as long as the nanowire's length L is much greater than the depth of the SiO₂ layer. Clearly, this is true for the nanowires examined here ($2\text{ }\mu\text{m} < L < 8\text{ }\mu\text{m}$). The suitability of the one-dimensional heat transport model was also confirmed by comparing predicted results with those from a fully three-dimensional simulation using commercial software (Comsol Multiphysics®). Figure S2a shows a schematic of the simulation domain, which included half of the GaN nanowire, one of the Au/Ti contacts, and a portion of the SiO₂/Si substrate. The color of each object indicates its room temperature thermal conductivity, the exact values of which are listed in Table S1. Note that a value of 6.0 W/m·K was assumed for the thermal conductivity of the SiO₂ layer. The use of this value is discussed below, although it is worth noting that at 6.0 W/m·K the value of the substrate thermal conductivity is approaching that of the nanowire, and thus the one-dimensional heat transport model may not be strictly valid.

Heat generation within the nanowire was estimated by simulating the electric current flow through the nanowire assuming a uniform electrical conductivity of 7430 S/m (a typical value for our samples based on electrical measurements). The electric potential was fixed at 4.15 V at the midplane surface of the nanowire (at the edge of the simulation domain), and the electric potential of the Au/Ti contact electrode was grounded at another edge of the simulation domain. The resulting heat generation is shown in Fig. S2b, which indicates that the predicted heat generation is approximately uniform over nearly all of the nanowire's length. The fact that the heat generation is highest immediately near the nanowire/metal junction is due to electric current constriction as current enters the nanowire.

Figure S2c contains a surface colormap of the predicted temperature rise due to the electrical heat generation shown in Fig. S2b and reveals that the temperature distribution in the nanowire is not strictly one-dimensional but varies somewhat throughout the nanowire cross-section. The corresponding temperature slice plot in Fig. S2d confirms this observation. The temperature profile predicted by the three-dimensional solution is compared with that of the one-dimensional model in Fig. S3. The solid black line corresponds to a one-dimensional numerical solution assuming a value of $47 \text{ W/mm}^2\cdot\text{K}$ for substrate thermal conductance per unit area G''_{nw-sub} , and the green 'x's represent the nanowire's temperature profile along its geometric centroid as predicted by the three-dimensional simulation. The good agreement between the two curves illustrates that the one-dimensional model is still useful even when the thermal conductivity of the SiO_2 layer is assumed to be as high as a value of $6.0 \text{ W/m}\cdot\text{K}$. The temperature of the nanowire's top edge and bottom surface ($y = z = 0$) as predicted by the three-dimensional simulation

is also shown in Fig. S3 (red and blue x's, respectively) and indicate that the maximum temperature drop across the nanowire cross-section is approximately 45 K.

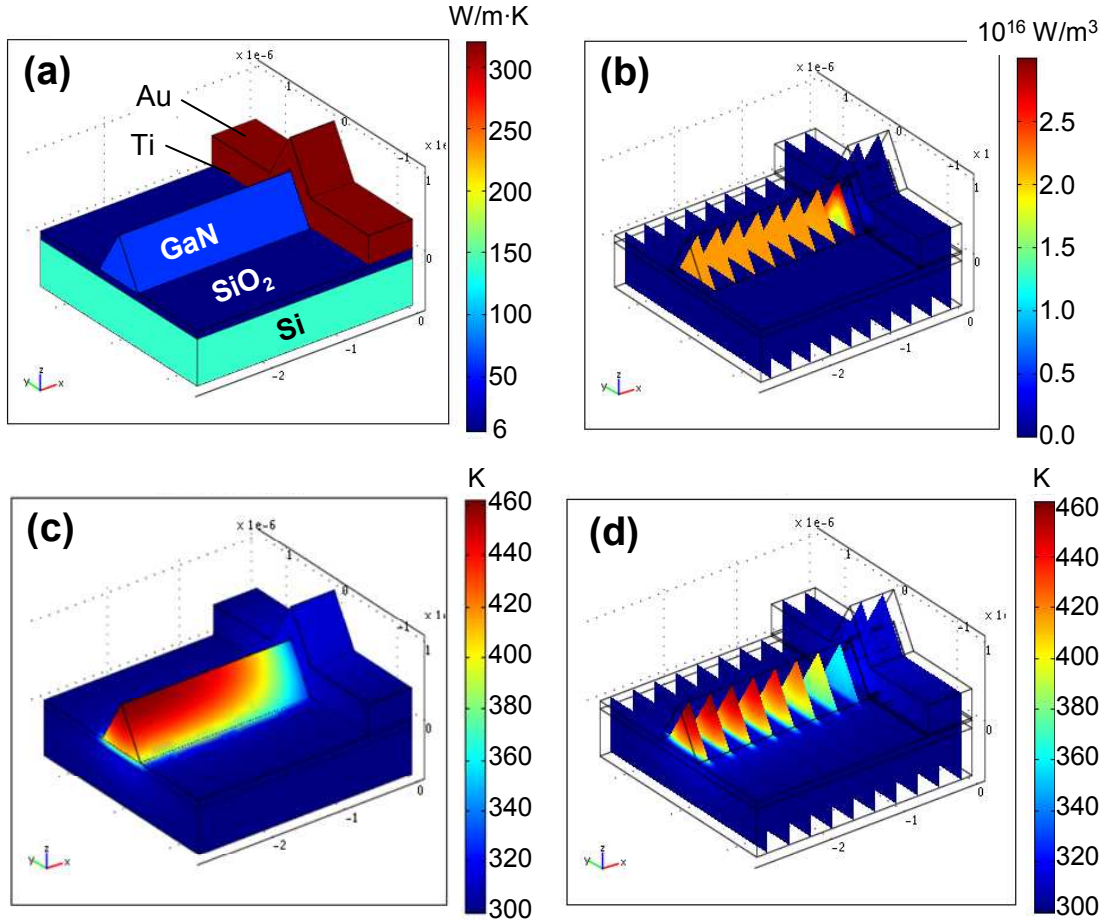


Figure S2. (a) Colormap of three-dimensional simulation domain showing room temperature thermal conductivities of individual components. (b) Predicted electrical heat generation at several domain cross-sections. (c) and (d) Predicted temperature rise on surface and at several domain cross-sections, respectively.

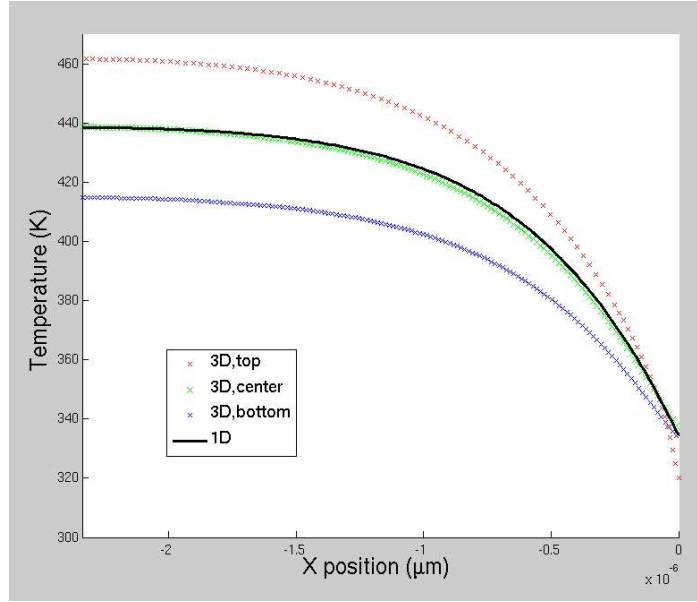


Figure S3. Comparison of temperature profiles predicted by the one- and three-dimensional simulations. The black line represents the one-dimensional prediction while the red, green, and blue ‘x’s represent the three-dimensional prediction at the nanowires top (apex), centroid, and bottom ($y = z = 0$).

Table S1. Parameter values employed in one- and three-dimensional simulations.

Nanowire length	4.7	μm
Nanowire width	0.68	μm
Nanowire thermal conductivity@300 K	60	$\text{W/m}\cdot\text{K}$
Nanowire electrical conductivity	7430	S/m
Total power dissipation	21.0	mW
Substrate temperature	300	K
Metal temperature (1-D simulation)	334.6	K
SiO_2 thermal conductivity	6.0	$\text{W/m}\cdot\text{K}$
Si thermal conductivity	140.0	$\text{W/m}\cdot\text{K}$
Au thermal conductivity	320.0	$\text{W/m}\cdot\text{K}$
Au electrical conductivity	$4.5\text{e}7$	S/m
Si temperature far from nanowire (3D simulation)	300	K

Validity of neglecting thermal radiation and convection

Heat dissipation per unit length of the nanowire is dominated by conduction both along the nanowire's axis and into the wafer substrate. This is easily shown by comparing the three modes of heat transfer. Heat dissipation per nanowire length by conduction into the substrate is given by

$$q'_{sub} = G''_{nw-sub} \cdot W \cdot (T - T_{sub}) \quad (S1)$$

while that by thermal radiation to the surroundings is

$$q'_{rad} = \varepsilon \sigma_{S-B} 2W (T^4 - T_{surr}^4) = 2Wh_{rad} (T - T_{surr}) \quad (S2)$$

and that by convection to ambient air is

$$q'_{conv} = 2Wh_{conv} (T - T_{amb}) \quad (S3)$$

In eq. S2, ε is the surface emissivity of the nanowire, σ_{S-B} is the Stefan-Boltzmann constant ($5.67 \cdot 10^{-8} \text{ W/m}^2 \cdot \text{K}^4$), T_{surr} is the temperature of the surroundings (300 K), and h_{rad} is the radiation heat transfer coefficient, equal to $\varepsilon \sigma_{S-B} (T + T_{sub}) (T^2 + T_{surr}^2)$. In eq. S3, h_{conv} is the convective heat transfer coefficient, and T_{amb} is the temperature of the ambient air (300 K).

Comparing eqs S1 and S2, it is observed that radiation can be neglected if $G''_{nw-sub} \gg 2h_{rad}$. Assuming that the emissivity ε is that of a blackbody (*i.e.*, equal to unity, the maximum value possible) and that the nanowire's maximum temperature is 1000 K, a value of approximately $0.0001 \text{ W/mm}^2 \cdot \text{K}$ is obtained for h_{rad} . This value is much less than the estimated value of G''_{nw-sub} , which is approximately $50 \text{ W/mm}^2 \cdot \text{K}$ (see Fig. 3); thus, the effects of thermal radiation can be safely neglected.

Similar to the above analysis, heat dissipation by convection can be neglected if $G''_{nw-sub} \gg 2h_{conv}$. Several approximate correlations based on either forced or natural convection are available for estimating the convective heat transfer coefficient h_{conv} . All the correlations the authors applied to estimate h_{conv} yielded similar results, and therefore a single example calculation is sufficient here. The convective heat transfer coefficient h_{conv} is estimated as¹

$$h_{conv} \approx \frac{k_{air}}{W} 0.664 (V_{air} L_{wafer} / \nu)^{1/2} (Pr)^{1/3} \left[1 - \left(1 - \frac{L_{wafer}}{W} \right)^{3/4} \right]^{2/3} \quad (S4)$$

where k_{air} is the thermal conductivity of air, V_{air} is the air velocity far above the wafer, L_{wafer} is the distance from the nanowire to the edge of the wafer, ν is the dynamic viscosity of air, and Pr is the Prandtl number of air. Equation S4 is valid for laminar flow over an isothermally heated section of an otherwise unheated flat plate and is therefore appropriate for a small heated nanowire resting on an unheated wafer. The wafer is located within a probe station that is partially open to laboratory air that has a velocity on the scale of 1 m/s. The distance from the nanowire to the edge of the wafer is on the scale of 1 cm, the thermal conductivity of air is approximately 0.05 W/m·K (650 K), the dynamic viscosity of air is approximately $6 \cdot 10^{-5}$ m²/s, and the Prandtl number of air is approximately 0.7, resulting in a value of approximately 0.001 W/mm²·K for h_{conv} . Thus, h_{conv} is also much less than G''_{nw-sub} , and convection is negligible relative to heat conduction into the substrate. We note that eq S4 is valid only for continuum-type flows and may overpredict the effects of convection because the mean free path of air molecules above the nanowire is on the scale of the nanowire's width.

Supplementary References

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- (1) Incropera, F. P.; DeWitt, D. P. *Fundamentals of Heat and Mass Transfer*, 5th ed.; Wiley: Hoboken, NJ, 2002, pg. 398.