Electro-Thermal Modeling Of A Gated-Graphene Device

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Abstract

The thermoelectric response of a nanoscale device can be characterized by measuring either the open-circuit thermovoltage or the closed-circuit thermocurrent. While theoretically equivalent through the device's conductance, the thermocurrent measurement offers significant practical advantages, including faster acquisition times and the ability to characterize high-impedance samples where voltage measurements are challenging. To derive the efficiency of the thermoelectric device, one needs precise knowledge of the temperature gradient (ΔT) across the active region.

This work presents a combined experimental and computational approach to validate the analysis of thermoelectric measurements on a gated graphene device. Although AC lock in techniques allow for sensitive detection of thermoelectric signals at the second harmonic (2ω), the temperature gradient (ΔT) is not directly measured on-chip. We therefore use a COMSOL Multiphysics® model to calculate ΔT and then quantitatively compare the simulated gradient with the ΔT extracted from the same device by fitting the gate dependent Seebeck coefficient using the Mott formula. Because the measurement is performed after the system has reached thermal equilibrium, the electronic and phononic temperatures are assumed to be equivalent (Te ≈ Tph). This allows for a direct comparison between the ΔT obtained from Mott fitting and the lattice-temperature gradient produced by the simulation. This comparison provides a self consistent, physics based validation of our experimental results.

Figures 1 a-b) show the device at the heart of this study, comparing the geometry of the COMSOL model with a false-colored SEM image of the actual fabricated device. To achieve this, we developed a custom 3D electro-thermal model using the AC/DC and Heat Transfer Modules. The model treats graphene as 0.335 nm thick 3D domain with anisotropic thermal properties to accurately capture its heat-spreading characteristics. The in-plane thermal conductivity was set to 1300 W/(m·K) based on recent first-principles calculations, while an out-of-plane conductivity of 0.01675 W/(m·K) was used to model the significant thermal boundary conductance (50 MW/(m²·K)) between the graphene and the platinum substrate [1, 2]. The model couples the Electric Current (ec) and Heat Transfer in Solids (ht) interfaces and uses a time-dependent study to apply an AC current at frequency ω, which generates Joule heat at 2ω. This is critical as our experiments isolate the thermoelectric signal at this second harmonic. The results of this thermal simulation are presented in Figure 2 d-f), which shows the time-dependent temperature distribution across the device and the trend as function of Iheater. The key quantitative check is given in Figure 2 d, which contrasts the COMSOL simulation at a base temperature of 100 K with the ΔT derived from the Mott fit. The model yields ΔTCOMSOL = 0.193 K, while the experiment gives ΔTMott = 0.261 K. Their close match demonstrates that the electro-thermal model faithfully captures the actual temperature gradient and confirms the reliability of the thermoelectric parameters extracted from harmonic measurements. Together, these results showcase the power of indirect harmonic thermoelectric measurements, validated by a physics based simulation, as a robust methodology for quantifying temperature gradients and assessing device performance in nanoscale systems.

Reference

[1] Han, Z., & Ruan, X. (2023). Thermal conductivity of monolayer graphene: Convergent and lower than diamond. Physical Review B, 108(12), L121412.
[2] Chen, J., et al. (2012). Interfacial Thermal Conductance of Graphene on Metals. Journal of Nanoscience and Nanotechnology, 12(1), 239-244.

Figures used in the abstract

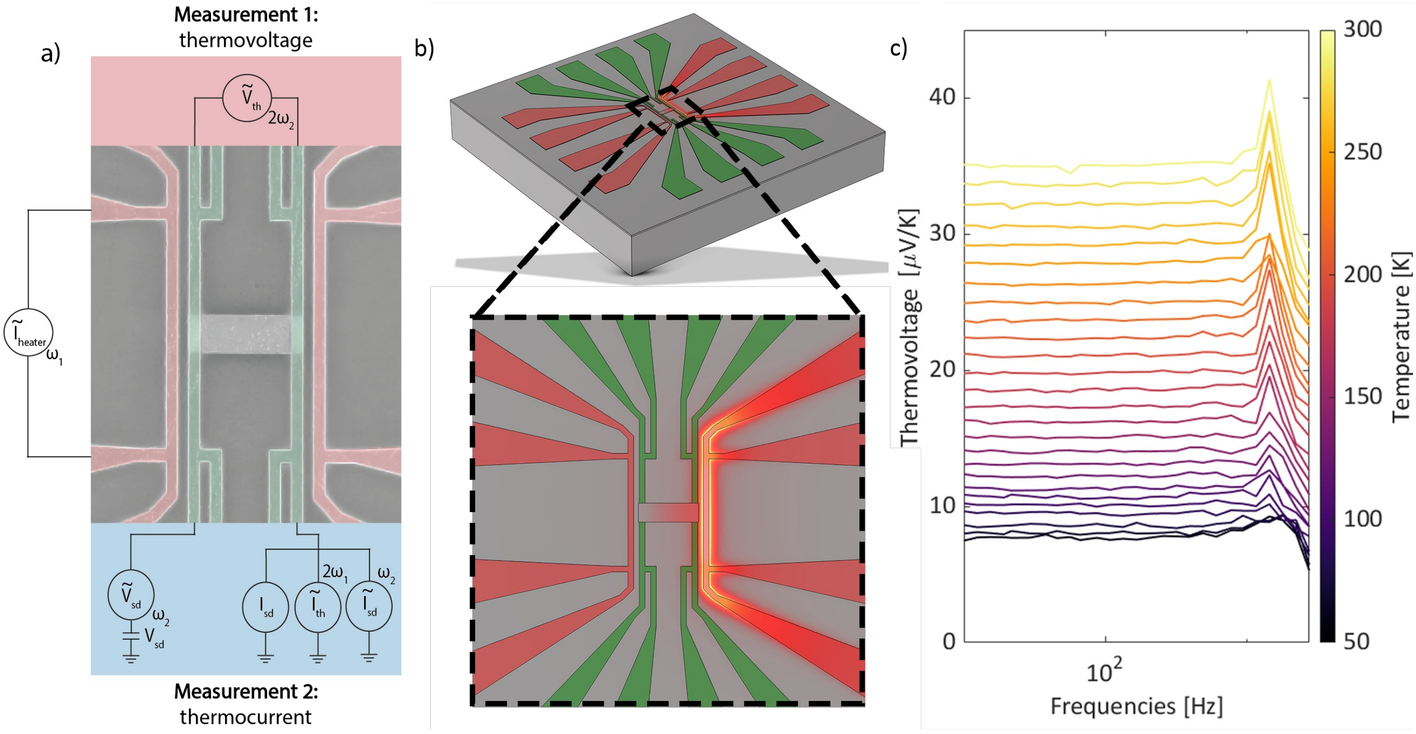

Figure 1 : Figure 1. Simulation and experiment overview. a) A false-colored SEM image of the fabricated device is overlaid with the measurement schematic. An AC current at frequency ω₁ is applied to the heater (red electrodes), and the resulting thermovoltage (Measu

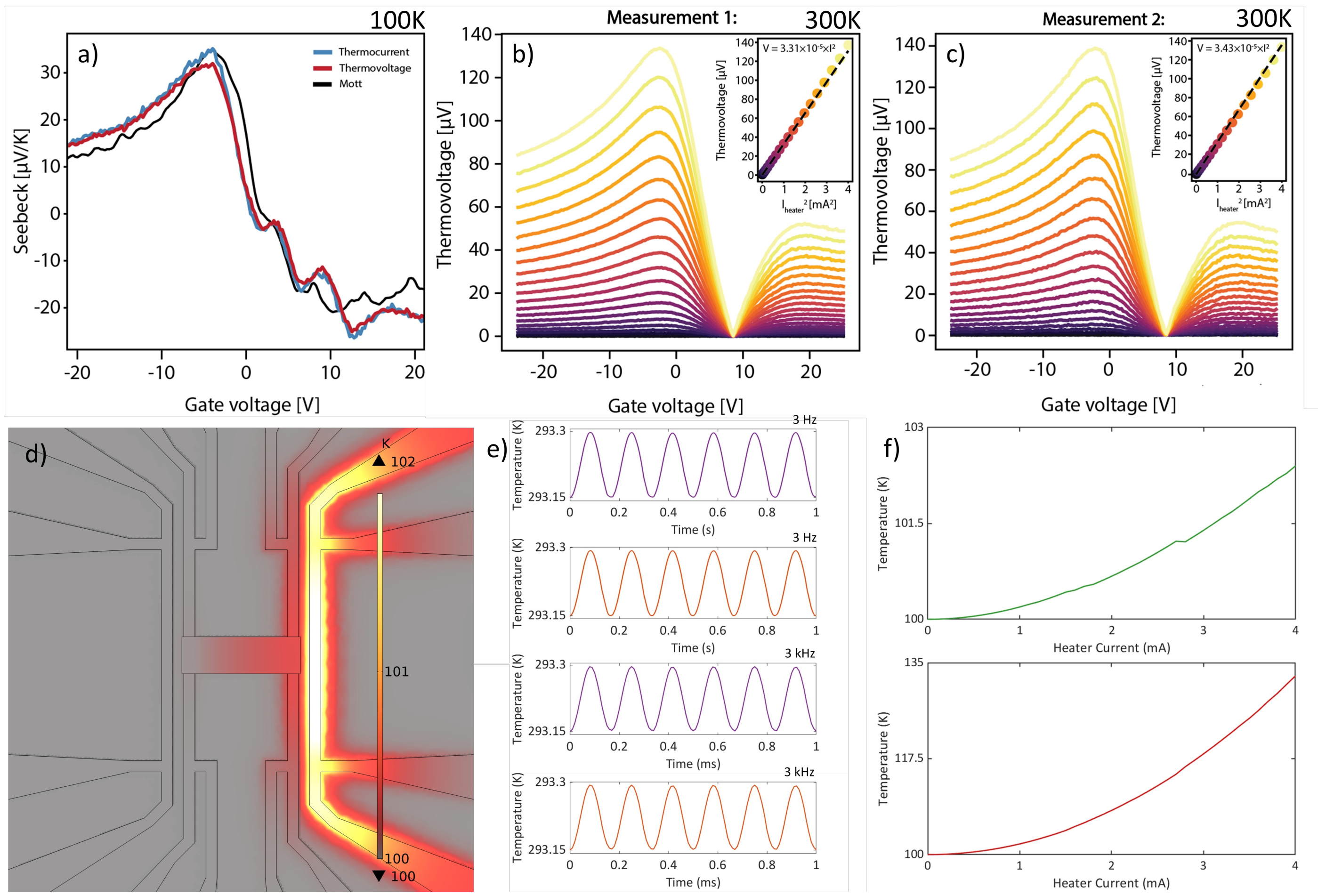

Figure 2 : Figure 2. Comparison between measured thermovoltage and theoretical prediction. a) At 100 K, the Seebeck coefficient measured directly (thermovoltage, red) and indirectly (thermocurrent, blue) shows excellent agreement with the Mott formula fit (black),