**Sample Shape and Boundary Dependence of Transverse Thermal Properties Measured through a Thermal Hall Bar**

Samuel Mumford,1,2 Tiffany Paul,1,3 Erik Kountz,1,2 and Aharon Kapitulnik1,2,3

1) Geballe Laboratory for Advanced Materials, Stanford University, Stanford CA, 94305, USA
2) Department of Physics, Stanford University, Stanford CA, 94305, USA
3) Department of Applied Physics, Stanford University, Stanford CA, 94305, USA

(Dated: 22 July 2020)

Despite increased interest in thermal Hall measurements for the analysis of insulating quantum materials, there remains large uncertainty in such measurements due to contact misalignment. In this paper, we propose that sample geometry and uncertain boundary conditions may account for uncertainty in the measurement of $D_{xy}$ or $\kappa_{xy}$. By running simple simulations in an open source finite-element solver, we demonstrate that measured $D_{xy}$ in a thermal Hall bar can be changed by a factor of order unity in samples with similar width and length. This geometric corrective factor depends on the distinction between uniform heat flow and constant temperature boundary couplings to a bath. Finally, sample geometry can be accounted for through simulation or by using more rectangular samples to make thermal Hall measurements more reliable and reproducible when the amplitude of $\kappa_{xy}$ is important.

---

**I. INTRODUCTION**

Measurement of the thermal Hall effect has emerged as a unique tool to investigate the nature of elementary excitations in solids, especially in response to the application of a magnetic field. Unlike the electric Hall response, a longitudinal temperature gradient may couple to a host of elementary excitations in both conductors and insulators such as spin or non-quasiparticle response, yielding unique transverse thermal response. Indeed, thermal Hall conductivity ($\kappa_{xy}$) measurements have become important in investigating magnetic insulators such as disordered or frustrated magnets and spin liquid magnons in kagome and pyrochlore lattices,

and it has been demonstrated that phonons also respond to a temperature gradient,

and may yield an unexpectedly large $\kappa_{xy}$.

Despite interest in thermal Hall measurements, there are large uncertainties and discrepancies in transverse thermal transport measurements. For a thermal Hall bar designed as in Fig. 1a, if the contacts used to measure the transverse temperature difference $\Delta T_i$ are misaligned, the longitudinal thermal gradient pollutes measurement of $\Delta T_i$ and the corresponding $\kappa_{xy}$ or $D_{xy}$. This familiar alignment uncertainty can account for an $\sim 20 - 50\%$ error in $\kappa_{xy}$ after antisymmetrization with magnetic field,

and limits measurement of small $\kappa_{xy}$ much as it does for small $\rho_{xy}$.

Beyond this familiar source of uncertainty, the temperature anchoring of thermal Hall bars makes boundary conditions uncertain and introduces a second source of measurement error not seen in voltage Hall bars. The differences in $\kappa_{xy}$ between ostensibly similar samples can be much larger than the statistical spread in data points, despite following similar temperature profiles.

In this paper, we propose through finite element simulation that such discrepancies may be attributed to geometric effects in thermal Hall bar measurements arising from the thermal boundary conditions. Such effects can change the measured $\kappa_{xy}$ by $\sim 50\%$ for square samples. As the geometric corrective factor depends only on one unitless parameter, thermal Hall measurements could be made with increased confidence by accounting for sample geometry either with simulation or experimental design changes.

---

**II. SIMULATION SETUP**

The heat diffusion equation can be written in frequency space for a heat source $g$ modulated at frequency $\omega$ as

$$i\omega T - \nabla \cdot (D \nabla T) = g(r) = \frac{Q}{c}.$$  

(1)

In order to address the effect of finite sample size on measurements of thermal diffusivity $D$, the temperature response of a sample was simulated using the open source finite element solver FEniCS. FEniCS allows for the implementation of linear differential equations in the weak form. Using test functions $v_1$ and $v_2$, separating the real and imaginary parts of $T$ and $g$, and integrating by parts in Eqn. 1 yields

$$\int -\omega T v_1 + \left( D \nabla T \right) \cdot \nabla v_1 + \omega T v_2 + \left( D \nabla T \right) \cdot \nabla v_2 dV = 0$$

(2)

$$= \int g_r v_1 + g_i v_2 dV$$

and boundary terms. Note that for a DC measurement, $\omega = T_i = g_i = 0$, giving

$$\int \left( D \nabla T \right) \cdot \nabla v_1 dV = \int g_r v_1 dV.$$  

(3)

Boundary conditions can be enforced implicitly or hard-coded into FEniCS simulation. Constant temperature boundary conditions are enforced through setting $v_1 = 0$ on the...
III. SAMPLE DIMENSION DEPENDENCE

For DC heat flow in the x-direction\cite{15},

\[
\frac{dT}{dx} = \frac{D_{xy}}{D_{xx}}.
\]  

(5)

Assuming uniform and constant heat flow, for a sample with y-dimensional or transverse width $w$, x-dimensional or longitudinal length $l$, and z-dimensional or magnetic flux-direction height $h$, $dT/dy = \Delta T_y/w$ and $dT/dx = \Delta T_x/l$. The $h$-
independent term is then
\[
\frac{\Delta T_y}{\Delta T_x} = \frac{w}{l} \frac{D_{xy}}{D_{xx}}.
\] (6)

This geometry is shown in Fig. 1.

To assess the effect of boundary uncertainty in the application of Eqn. 6, transverse thermal transport was simulated under the boundary conditions of:

- Uniform heat flow on the top and bottom surfaces. This is the standard assumption in a thermal Hall bar leading to Eqn. 6.
- Constant temperature boundary conditions for the top and bottom surfaces. This may be more accurate physically if a sample is directly attached to a temperature controlled substrate.
- Constant heat flow on the top surface and constant temperature on the bottom surface. This is analogous to a resistive heater on one surface and temperature anchoring to a cold bath on the bottom.

### A. Constant Heat Flow Boundary Conditions

As seen in Fig. 2, the simulated \(D_{xy}\) values match the true value outside of the extreme sample boundaries when the standard boundary conditions of uniform heat flow are enforced. The edge values are strongly asymmetric on the top and bottom surfaces and depend on simulation mesh size. Such dependence on simulation parameters suggests that deviations from the expected behavior arise from simulation error and that agreement with Eqn. 6 would improve with increased computing power.

Note that simulating Eqn. 4 is analogous to simulating transport in an electrical Hall bar in which the electrical analogue of Eqn. 6 is known to produce reliable results. Correspondingly, demonstrating that Eqn. 6 is reproduced in simulation with uniform heat flow is a necessary step in establishing simulation reliability. The observed agreement demonstrates that the FEniCS simulations reproduce the known experimental behavior of \(D_{xy}\) in a Hall bar to within 10% outside of extrema and benchmarks simulation accuracy.

### B. Constant Temperature Boundary Conditions

Experimental thermal Hall bars may not respect the assumed boundary conditions of uniform heat flow used for Eqn. 6. Instead, the top surface is placed in contact with a resistive heater on one surface and temperature anchoring to a cold bath on the bottom. As seen in Fig. 2, the simulated \(D_{xy}\) values match the true value outside of the extreme sample boundaries when the standard boundary conditions of uniform heat flow are enforced. The edge values are strongly asymmetric on the top and bottom surfaces and depend on simulation mesh size. Such dependence on simulation parameters suggests that deviations from the expected behavior arise from simulation error and that agreement with Eqn. 6 would improve with increased computing power.

Note that simulating Eqn. 4 is analogous to simulating transport in an electrical Hall bar in which the electrical analogue of Eqn. 6 is known to produce reliable results. Correspondingly, demonstrating that Eqn. 6 is reproduced in simulation with uniform heat flow is a necessary step in establishing simulation reliability. The observed agreement demonstrates that the FEniCS simulations reproduce the known experimental behavior of \(D_{xy}\) in a Hall bar to within 10% outside of extrema and benchmarks simulation accuracy.

![Profile of the ratio of the observed \(D_{xy}\) to the true value \(D_{xy,0} = 0.001\) w²/s with uniform heat flow on the top and bottom surfaces at \(x = 0\) and \(x = 3\) depending on the position of measurement of \(\Delta T_x\), \(x\). Note that outside of the top and bottom 10% of the sample, the measured and true values match to within the simulation uncertainty. Data is simulated with \(D_{xx} = D_{yy} = D_{zz} = 1\) w²/s and \(h = 0.2\) u.](image-url)

Highly non-uniform heat flow near the boundary. Such boundary conditions are incompatible with Eqn. 6. Instead, the top surface is placed in contact with a resistive heater on one surface and temperature anchoring to a cold bath on the bottom. As seen in Fig. 2, the simulated \(D_{xy}\) values match the true value outside of the extreme sample boundaries when the standard boundary conditions of uniform heat flow are enforced. The edge values are strongly asymmetric on the top and bottom surfaces and depend on simulation mesh size. Such dependence on simulation parameters suggests that deviations from the expected behavior arise from simulation error and that agreement with Eqn. 6 would improve with increased computing power. Correspondingly, demonstrating that Eqn. 6 is reproduced in simulation with uniform heat flow is a necessary step in establishing simulation reliability. The observed agreement demonstrates that the FEniCS simulations reproduce the known experimental behavior of \(D_{xy}\) in a Hall bar to within 10% outside of extrema and benchmarks simulation accuracy.

![Profile of the ratio of the observed \(D_{xy}\) to the true value \(D_{xy,0} = 0.001\) w²/s with uniform heat flow on the top and bottom surfaces at \(x = 0\) and \(x = 3\) depending on the position of measurement of \(\Delta T_x\), \(x\). Note that outside of the top and bottom 10% of the sample, the measured and true values match to within the simulation uncertainty. Data is simulated with \(D_{xx} = D_{yy} = D_{zz} = 1\) w²/s and \(h = 0.2\) u.](image-url)
FIG. 3. Profile of the ratio of the observed $D_{xy}$ to the true value $D_{xy,0} = 0.001 \text{ u}^2/\text{s}$ with $T = T_0$ on the bottom surface and $T = T_0 + 1$ on the top surface at $x = 3 \text{ u}$ depending on the position of measurement of $\Delta T_y$, $x$. a) Shown for $w = 0.3 \text{ u}$, note that the observed value has minimal positional dependence and reasonable agreement with the true value if $z > w$ from the top of bottom boundary. b) Shown for a variety of widths ranging from $w = 0.1l$ to $w = l$. The error in $D_{xy}$ measurement is $\sim 50\%$ for square samples even if measured at the optimal point. c) Shown for a variety of $w$ as a function of $x/w$. If $w < l$ and the top and bottom boundary contributions do not interact, the error dependence is largely determined by the unitless parameter $x/w$. Note that $w < 0.5l$ so that the contribution of each boundary can be isolated.

FIG. 4. Profile of the ratio of the observed $D_{xy}$ to the true value $D_{xy,0} = 0.001 \text{ u}^2/\text{s}$ with $T = T_0$ on the bottom surface and $T = T_0 + 1$ on the top surface at $x = 3 \text{ u}$. a) Measured at a variety of sample heights $h$. The $h$ dependence is negligible compared to the $w$ dependence and may be attributed to slightly different simulation mesh densities with different surface area to volume ratios. b) Measured at different longitudinal thermal diffusivities $D$. As expected, there is no evidence of $D$ dependence or a hidden diffusivity-based length scale.
length scales associated with the problem and that geometric corrections are determined by the sample lateral dimensions. The D and h-independence of the contact placement based error simplifies the problem of simulating for a corrective geometric factor and confirms simulation accuracy.

C. Mixed Boundary Conditions

Finally, simulations of a blended boundary condition with constant heat flow on the top surface and set temperature on the bottom surface exhibit the isolated boundary correction from one surface. Such a condition is closest to samples which are connected to a resistive heater on one end and firmly anchored to a constant temperature base on the other. As seen in the bottom surface exhibit the isolated boundary correction to a constant temperature surfaces, the viable measurement region of the top boundary D_{xy} with sample size. In contrast, the length scale of the bottom boundary contribution scales with the sample width. This is observed for a variety of sample widths and two forms of sample heating in Fig. 5a and b.

The viable range of w/l may also be extended even if only one surface can exhibits uniform heat flow. Comparing the D_{xy} response in Fig. 3 and Fig. 5 for samples with two constant temperature surfaces, the viable measurement region must be at \( \alpha > w \) from both surfaces and accurate measurement can only be performed with \( w < 0.3l \). In contrast, with only one constant temperature surface data may be taken with \( w \lesssim 0.5l \) provided observations are made above the sample midpoint.

IV. SUMMARY

The above discussion yields important guidelines for the measurement of thermal Hall coefficient, especially when the magnitude of the effect is important.

- Sample geometry and contact placement can significantly effect the measured \( D_{xy} \) or \( \kappa_{xy} \) in laterally square samples. As such an error is \( D_{xy} \)-independent, it would not be accounted for through antisymmetrization with magnetic field and is difficult to correct for.

- Rectangular samples with \( w < 0.3l \) should produce more consistent measurements of transverse thermal properties regardless of the thermal anchoring method. This condition is commonly met in \( \kappa_{xy} \) measurement where the amplitude of the signal is important and sample dimensions are listed.

- A geometric corrective factor can be simulated easily once per sample and used to increase confidence in the reproducibility of transverse thermal transport properties between samples if boundary conditions are known.

In conclusion, as theories become more detailed with actual material parameters used for comparison to experiments, it is important that experimental data is stated accounting for possible sample geometric error. Unlike electrical Hall bars with patterned contacts and current sources, there are a variety of methods used to control heat flow and temperature in thermal Hall bars. As boundary conditions can create large corrective factors for square samples, the chosen contact method and sample shapes are important elements in thermal Hall measurement.

1. M. Hirschberger, J. W. Krizan, R. J. Cava, and N. P. Ong, “Large thermal Hall conductivity of neutral spin excitations in a frustrated quantum magnet,” *Science* **348**, 106–109 (2015), https://science.sciencemag.org/content/348/6230/106.full.pdf

2. K. Sugii, M. Shimozawa, D. Watanabe, Y. Suzuki, M. Halimi, N. Kamiata, Y. Matsumoto, S. Nakatsuji, and M. Yamashita, “Thermal Hall effect in a phonon-glass ba2ucusbo2,” *Phys. Rev. Lett.* **118**, 145902 (2017).

3. D. Watanabe, K. Sugii, M. Shimozawa, Y. Suzuki, T. Yajima, H. Ishikawa, Z. Hiroi, T. Shibayachi, Y. Matsuda, and M. Yamashita, “Emergence of non-trivial magnetic excitations in a spin-liquid state of kagome volborthite,” *Proceedings of the National Academy of Sciences* **113**, 5653–5657 (2016), https://www.pnas.org/content/113/31/5653.full.pdf

4. Y. Kasahara, T. Ohnishi, Y. Mizukami, O. Tanaka, S. Ma, K. Sugii, N. Kurita, H. Tanaka, J. Nasu, Y. Motome, and et al., “Majorana quantization and half-integer thermal quantum Hall effect in a kagome spin liquid,” *Nature* **559**, 227–231 (2018).

5. Y. Kasahara, K. Sugii, T. Ohnishi, M. Shimozawa, M. Yamashita, N. Kurita, H. Tanaka, J. Nasu, Y. Motome, T. Shibayachi, and et al., “Unusual thermal hall effect in a kitaev spin liquid candidate nucl3,” *Physical Review Letters* **120** (2018), 10.1103/physrevlett.120.217205.

6. H. Doki, M. Akazawa, H.-Y. Lee, J. H. Han, K. Sugii, M. Shimozawa, N. Kawashima, M. Oda, H. Yoshida, and M. Yamashita, “Spin thermal hall conductivity of a kagome antiferromagnet,” *Phys. Rev. Lett.* **121**, 097203 (2018).

7. R. Henrich, M. Roslova, A. Isavea, T. Doert, W. Brenig, B. Büchner, and C. Hess, “Large thermal hall effect in α-rutile: Evidence for heat transport by kitaev-heisenberg paramagnons,” *Phys. Rev. B* **99**, 085136 (2019).

8. M. Hirschberger, R. Chisnell, Y. S. Lee, and N. P. Ong, “Thermal hall effect of spin excitations in a kagome magnet,” *Phys. Rev. Lett.* **115**, 106603 (2015).

9. T. Ideue, Y. Onose, H. Katsura, Y. Shiomi, S. Ishiwata, N. Nagaosa, and Y. Tokura, “Effect of lattice geometry on magnon hall effect in ferromagnetic insulators,” *Phys. Rev. B* **85**, 134411 (2012).

10. Y. Onose, T. Ideue, H. Katsura, Y. Shiomi, N. Nagaosa, and Y. Tokura, “Observation of the magnon hall effect,” *Science* **329**, 297–299 (2010), https://science.sciencemag.org/content/329/5989/297.full.pdf

11. A. V. Inyushkin and A. N. Taldenkov, “On the phonon hall effect in a paramagnetic dielectric,” *JEPT Letters* **86**, 379–382 (2007).

12. C. Strohm, G. L. J. A. Rikken, and P. Wyder, “Phenomenological evidence for the phonon hall effect,” *Phys. Rev. Lett.* **95**, 155901 (2005).

13. X. Li, B. Fauqué, Z. Zhu, and K. Behnia, “Phonon thermal hall effect in strontium titanate,” *Phys. Rev. Lett.* **124**, 105901 (2020).

14. M. S. Aftes, J. Blecha, J. Hake, A. Johansson, B. Kehlet, A. Logg, C. Richardson, J. Ring, M. E. Rognes, and G. N. Wells, “The fenics project version 1.5,” *Archive of Numerical Software* **3** (2015), 10.11588/anl.2015.102055.

15. A. Logg, G. N. Wells, and J. Hake, “Dolfin: a c++/python finite element library,” in *Automated Solution of Differential Equations by the Finite Element Method, Volume 84 of Lecture Notes in Computational Science and Engineering*, edited by A. Logg, K.-A. Mardal, and G. N. Wells (Springer, 2012) Chap. 10.

16. G. Grisonnanche, F. Lalande, S. Dufour-Beauséjour, M. Matusiak, S. Badoux, F. P. Tafti, B. Michon, A. Riepel, O. Cyr-Choinière, J. C. Baglo, B. J. Ramsaw, R. Liang, D. A. Bonn, W. N. Hardy, S. Krämer, D. Lebeuf, D. Graf, N. Doiron-Leyraud, and L. Taillefer, “Wiedemann-franz law in the underdoped cuprate superconductor yba2cu3o7,” *Phys. Rev. B* **93**, 064513 (2016).

17. H.-L. Kim, M. J. Coak, J. C. Baglo, K. Murphy, R. W. Hill, M. Sutherland, M. C. Hatnean, G. Balakrishnan, and J.-G. Park, “Modular thermal hall effect measurement setup for fast-turnaround screening of materials over
FIG. 5. a) Profile of the ratio of the observed $D_{xy}$ to the true value with $T = T_0$ on the bottom surface and $dT/dz = \alpha K/u$ on the top surface at $z = 3 \, u$. The constant $\alpha$ is selected so that the maximum temperature in the sample is 1 K. b) Modeling the input heat as a heater with an arbitrary penetration depth of 0.05 $u$. Note that this introduces a second length-scale to the problem, making the boundary form more complex. However, such an assumption makes simulation results more consistent between different finite element solver mesh densities.

wide temperature range using capacitive thermometry,” Review of Scientific Instruments 90, 103904 (2019).

18 X. Li, L. Xu, L. Ding, J. Wang, M. Shen, X. Lu, Z. Zhu, and K. Behnia, “Anomalous nernst and righi-leduc effects in mnsn: Berry curvature and entropy flow,” Phys. Rev. Lett. 119, 056601 (2017).

19 L. Xu, X. Li, X. Lu, C. Collignon, H. Fu, J. Koo, B. Fauqué, B. Yan, Z. Zhu, K. Behnia, and et al., “Finite-temperature violation of the anomalous transverse wiedemann-franz law,” Science Advances 6 (2020), 10.1126/sci-adv.aaz3522.