SCHOOL of ENGINEERING & APPLIED SCIENCE

Thermal transport in UWBG materials and interfaces: Challenges in measurements and understanding

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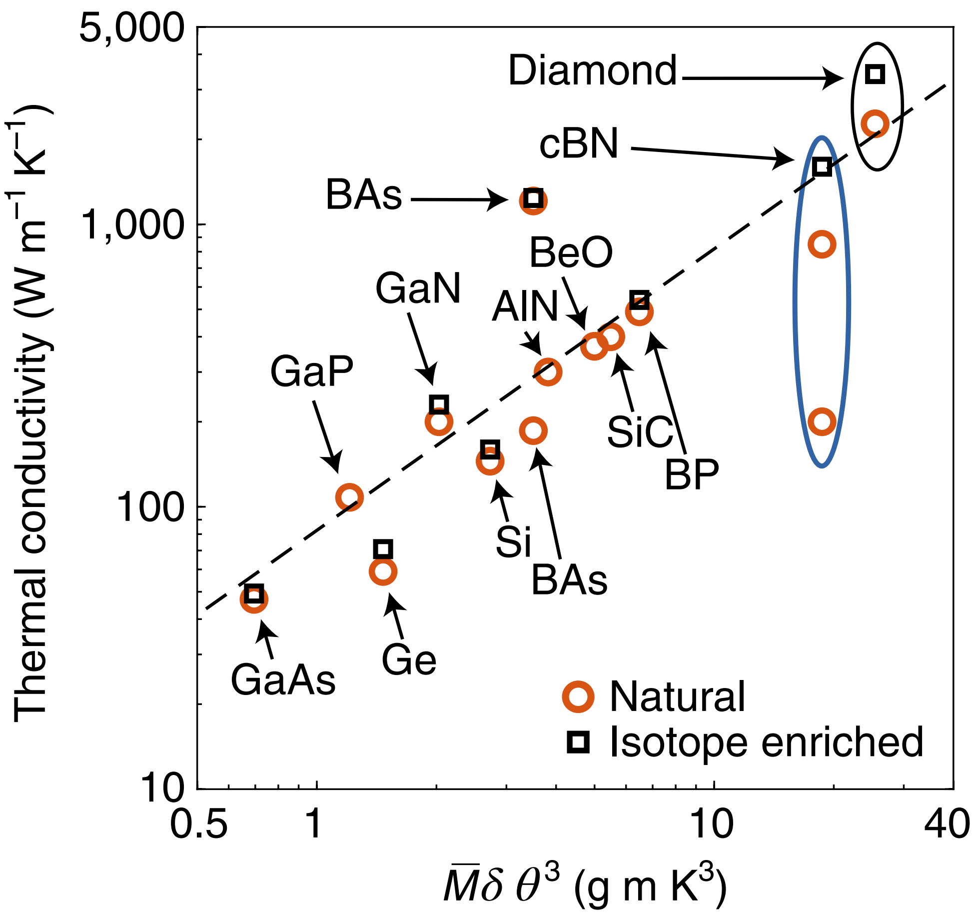
AT THE UNIVERSITY OF VIRGINIA

Thermal conductivity of materials

How do you make a great thermal conductor?



$$\kappa = \frac{1}{3}Cv\lambda = \frac{1}{3}Cv_g^2\tau$$

High κ

- Stiff, light mass, small unit cell, no defects,

Low κ

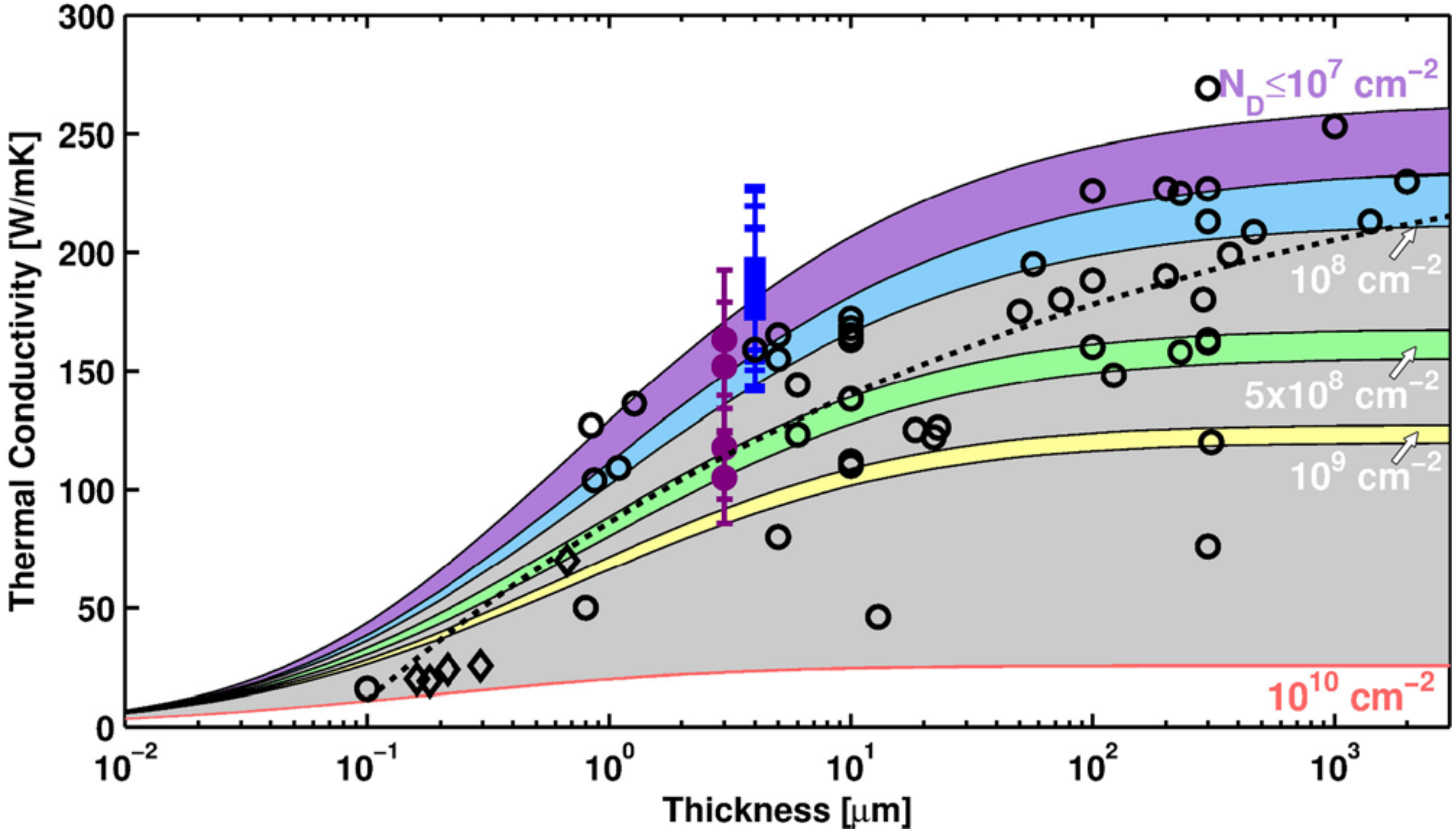
- Soft, heavy mass, large unit cell, complex unit cell, mass/chemical heterogeneities

Giri and Hopkins, *Nature Materials* **19**, 482

Nanoscale heat transfer of materials

But defects and interfaces impact κ

Ex: the case of GaN thin films



Beechem, *et al. J. Appl. Phys.* **120**, 095104

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Marko Tadjer
Travis Anderson

Georgia Tech
W. Alan Doolittle

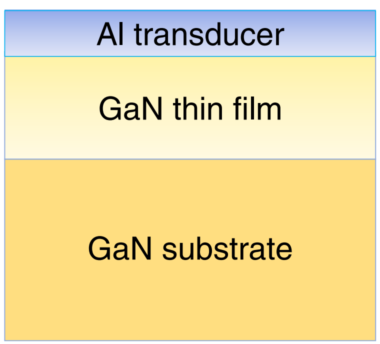
MIT
Asegun Henry

The importance of low defects films

Homoepitaxially grown GaN films exhibit exceptionally larger thermal conductivities

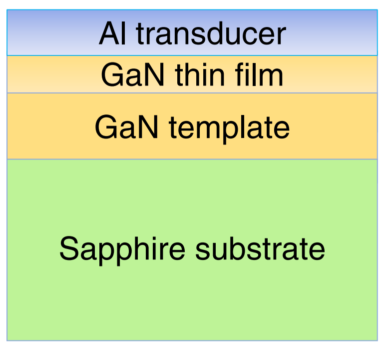
Hite
NRL

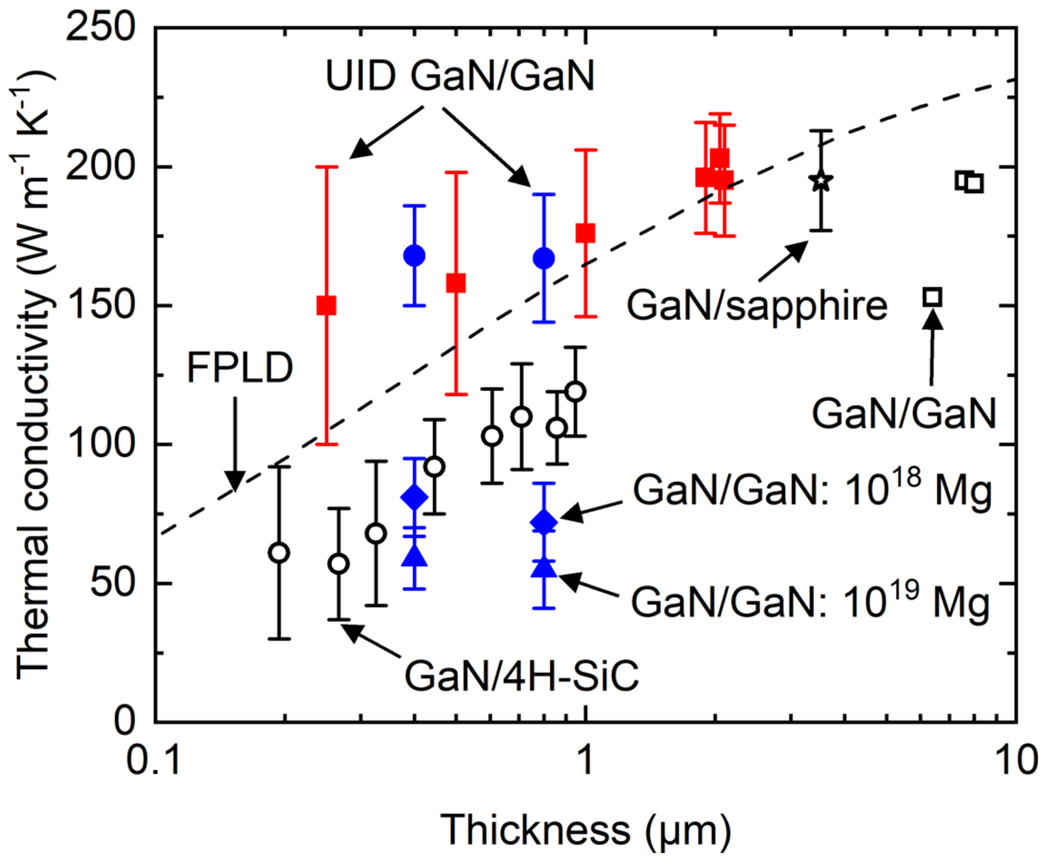
(a) MOCVD-grown



Doolittle
Ga Tech

(b) MBE-grown



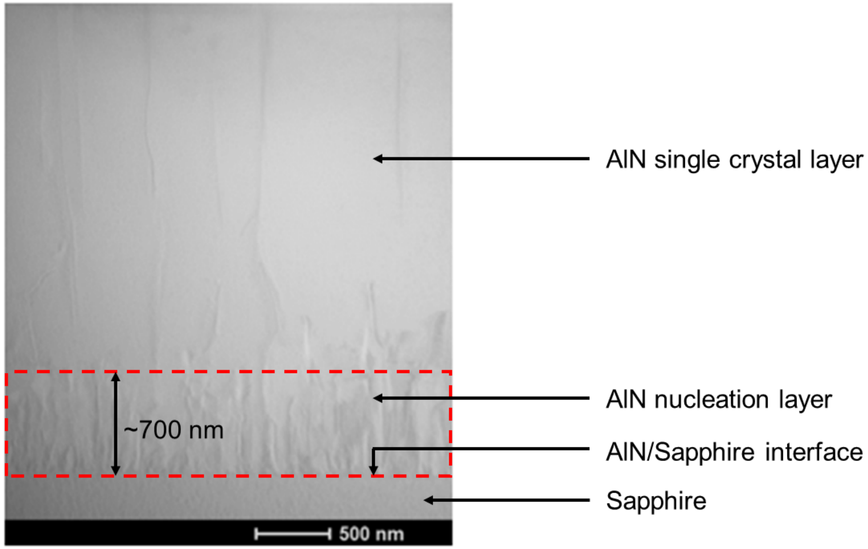


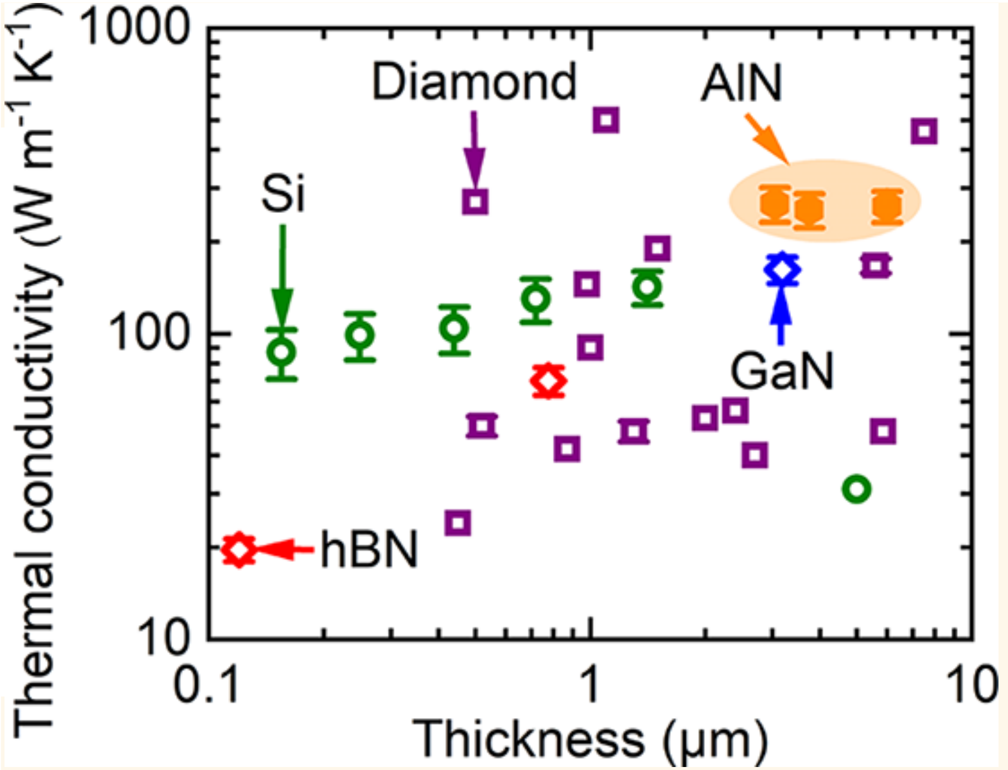
Koh, *et al. Phys. Rev. Mat.* **5**, 104604

The importance of low defects films

Exceptionally high *in plane* thermal conductivity of AlN films grown on sapphire substrates

Kahn
U. South Carolina





Hoque, *et al. ACS Nano* **15**, 9588

Goals for talk today: Major technical challenges in measurement and understanding of electron and phonon transport across WBG and UWBG interfaces

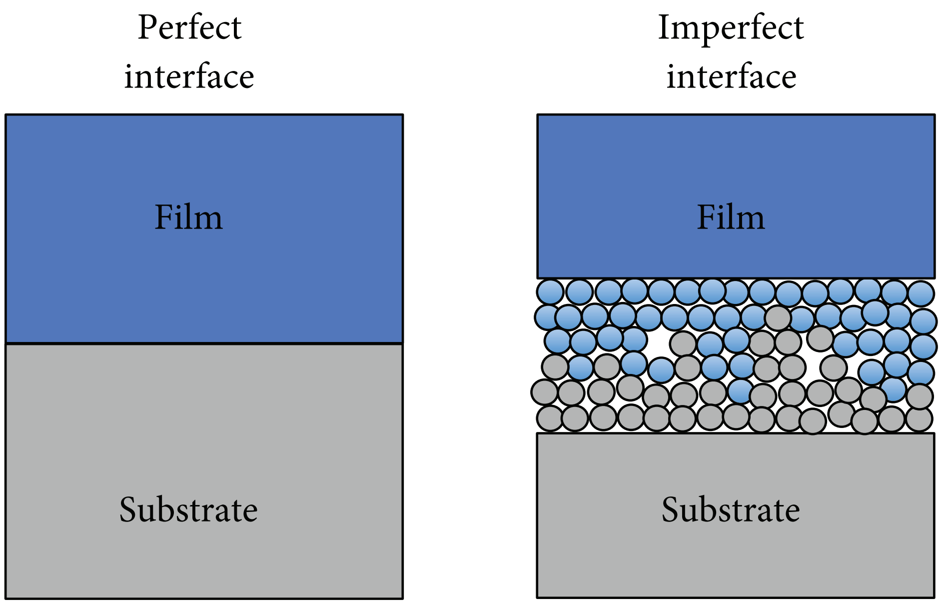
- Technical challenge – **Interfaces**: Designing interfaces to reduce TBR
  - Can we move beyond intrinsic phonon limitations in materials? *The "interfacial modes" and the "superlattice modes"*
  - Can we create new pathways for heat flow? *Electron "thermal short circuits" and thermal diodes*

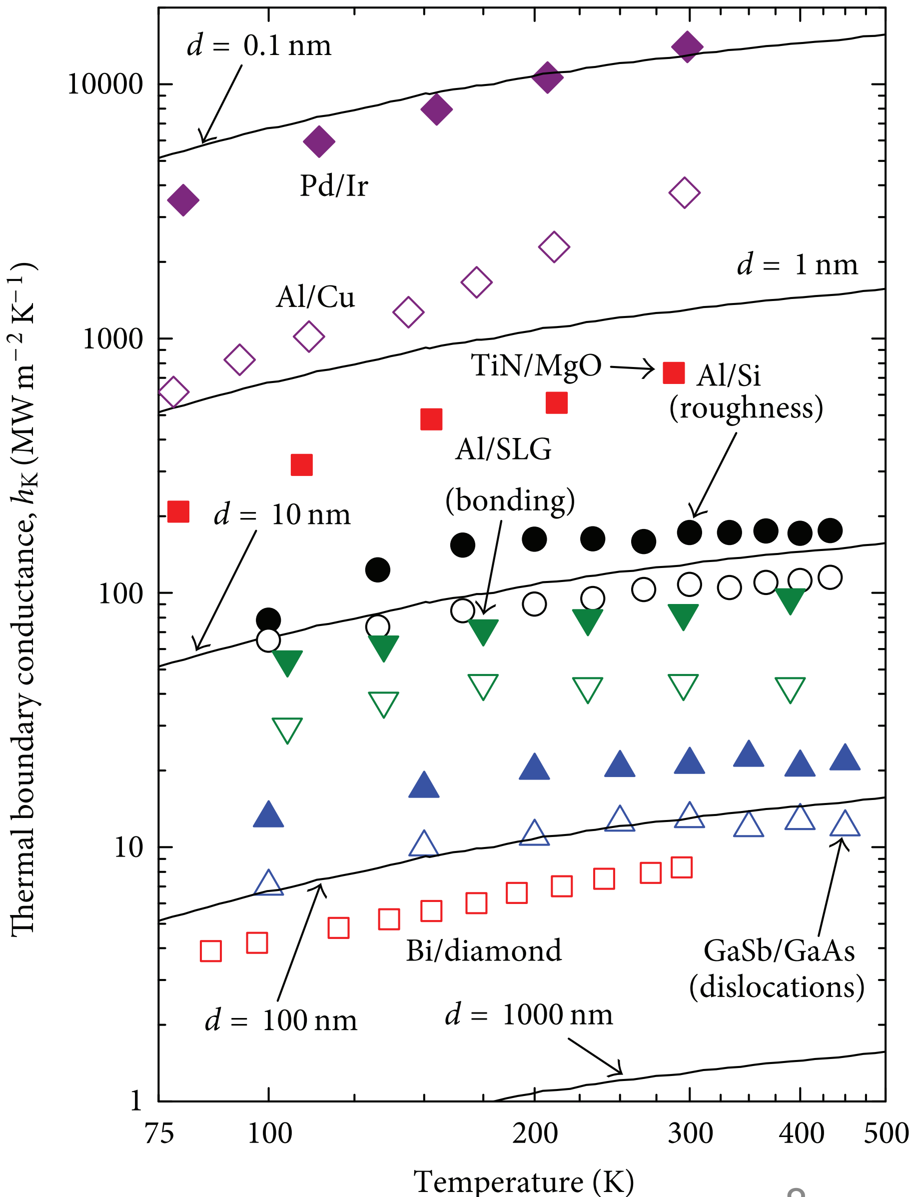
- Technical challenge – **Measurements**: Thermal conductivity and TBR measurements at device relevant length scales
  - Thermoreflectance-based techniques offer current state of the art
  - Limitations for measuring certain device-scale resistances
  - Need for turn-key thermal conductivity measurement tool for thin films that dos not require expert in thermoreflectance

Major technical challenge: thermal boundary resistance

$$q = h_K \Delta T = \frac{1}{R_K} \Delta T$$

Interfacial quality and chemistry matters



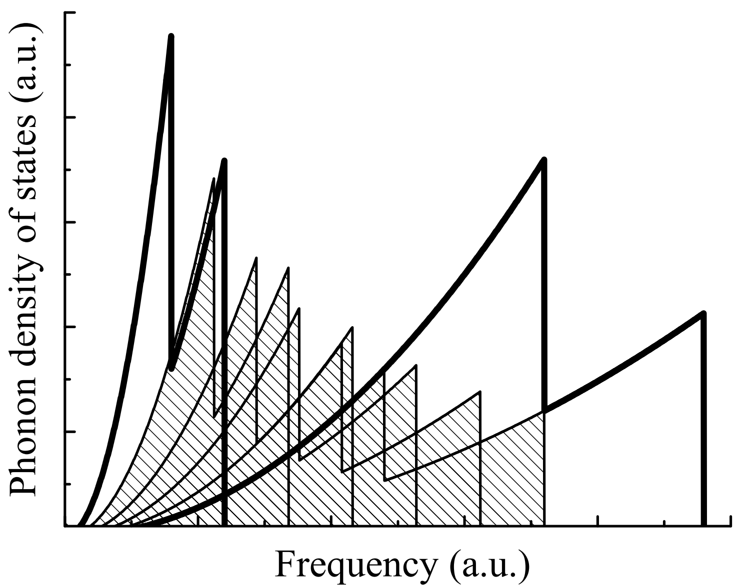


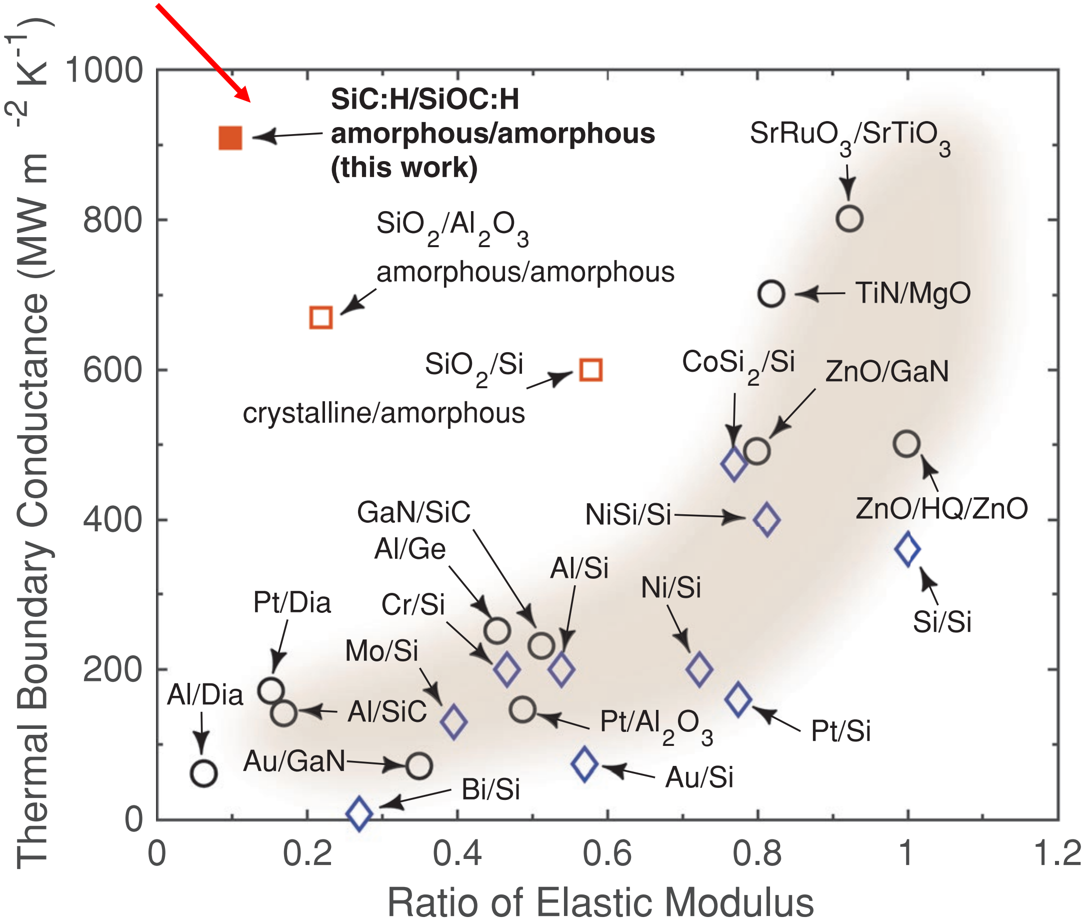
ISRN Mech. Eng. **2013**, 682586
Adv. Func. Mat. **30**, 1903857
Ann. Rev. Mat. Sci. **46**, 433

Intrinsic limitations from the "phonon mismatch" picture

Why aren't these materials restricted by same phononic mismatch trends?

Phonon density of states mismatch can intrinsically limit TBC

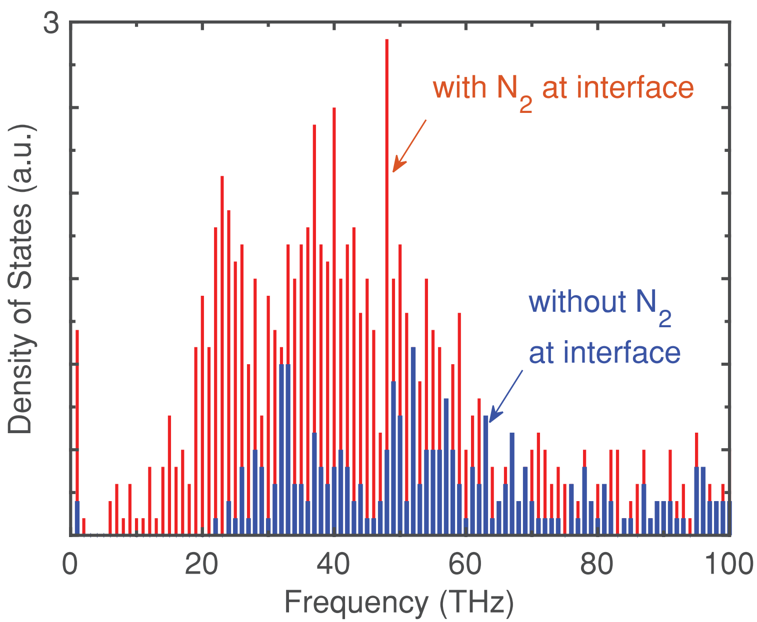


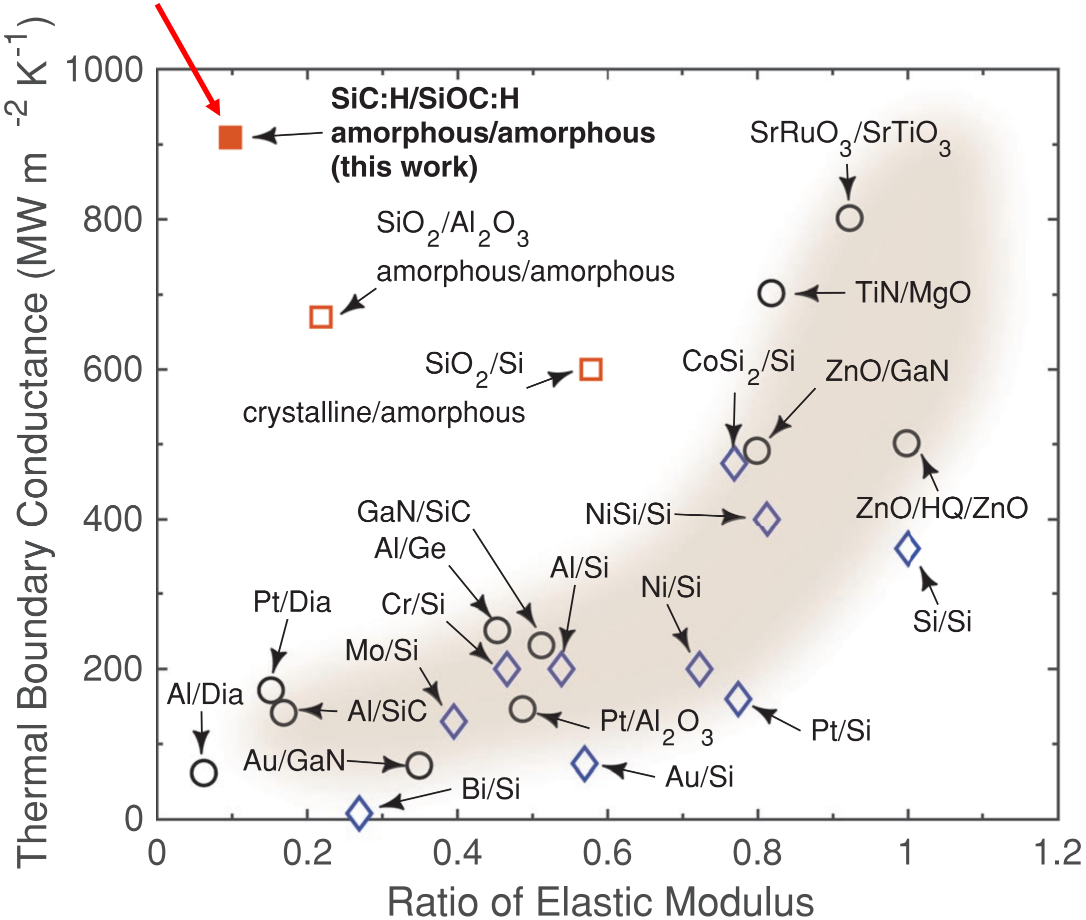


Giri *et al. Adv. Mat.* **30**, 1804097

Intrinsic limitations from the "phonon mismatch" picture

Interfacial defects can enhance thermal transport across interfaces

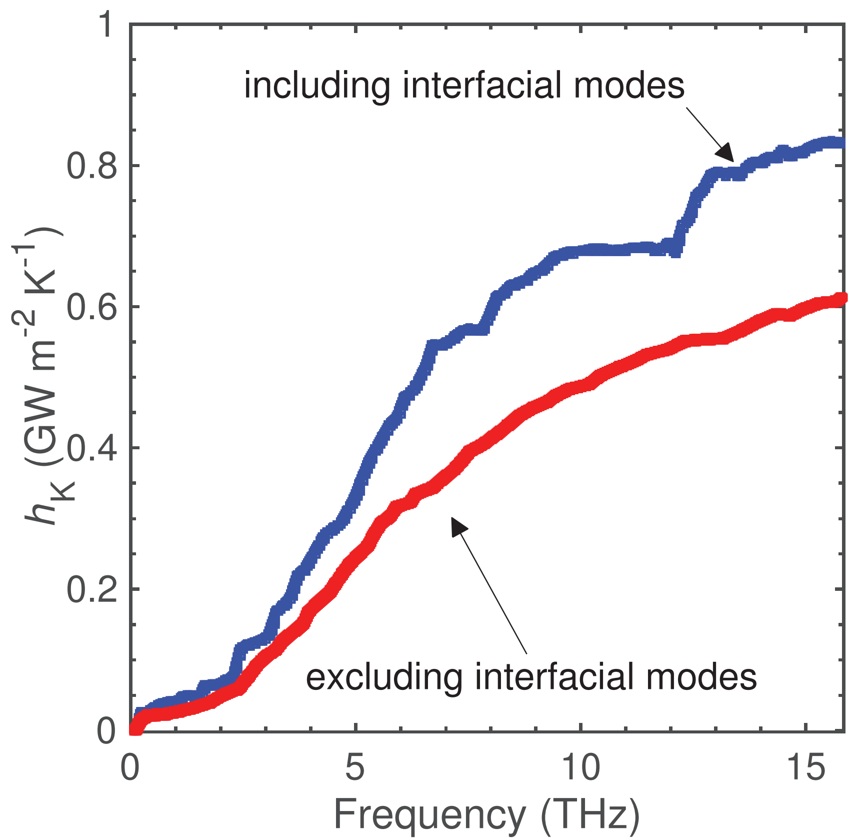




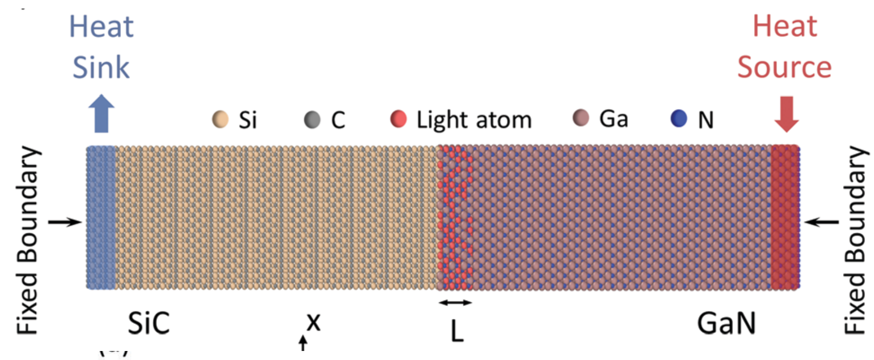
Giri *et al. Adv. Mat.* **30**, 1804097

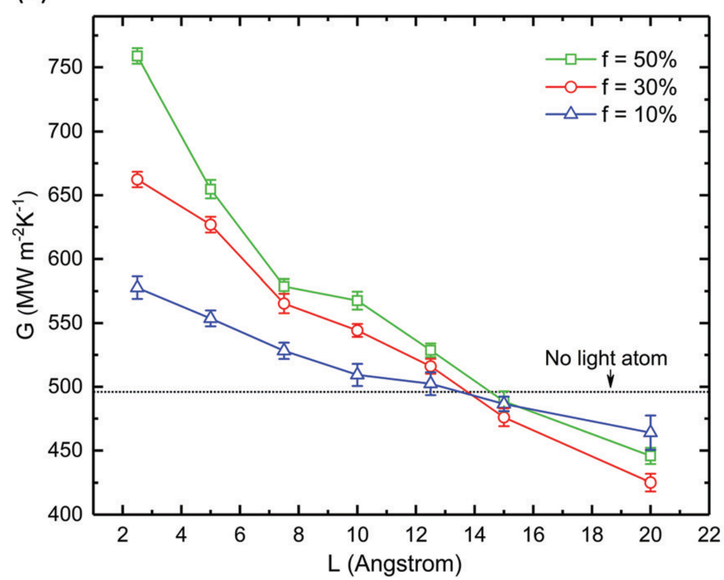
Interfacial modes can enhance TBC/reduce TBR

And interfacial defects can control the population and density of states of these modes



Gordiz and Henry,
J. Appl. Phys. **119**, 015101

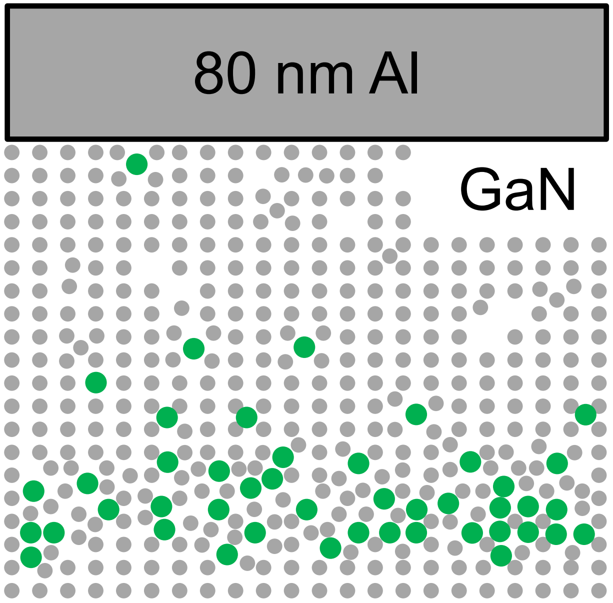




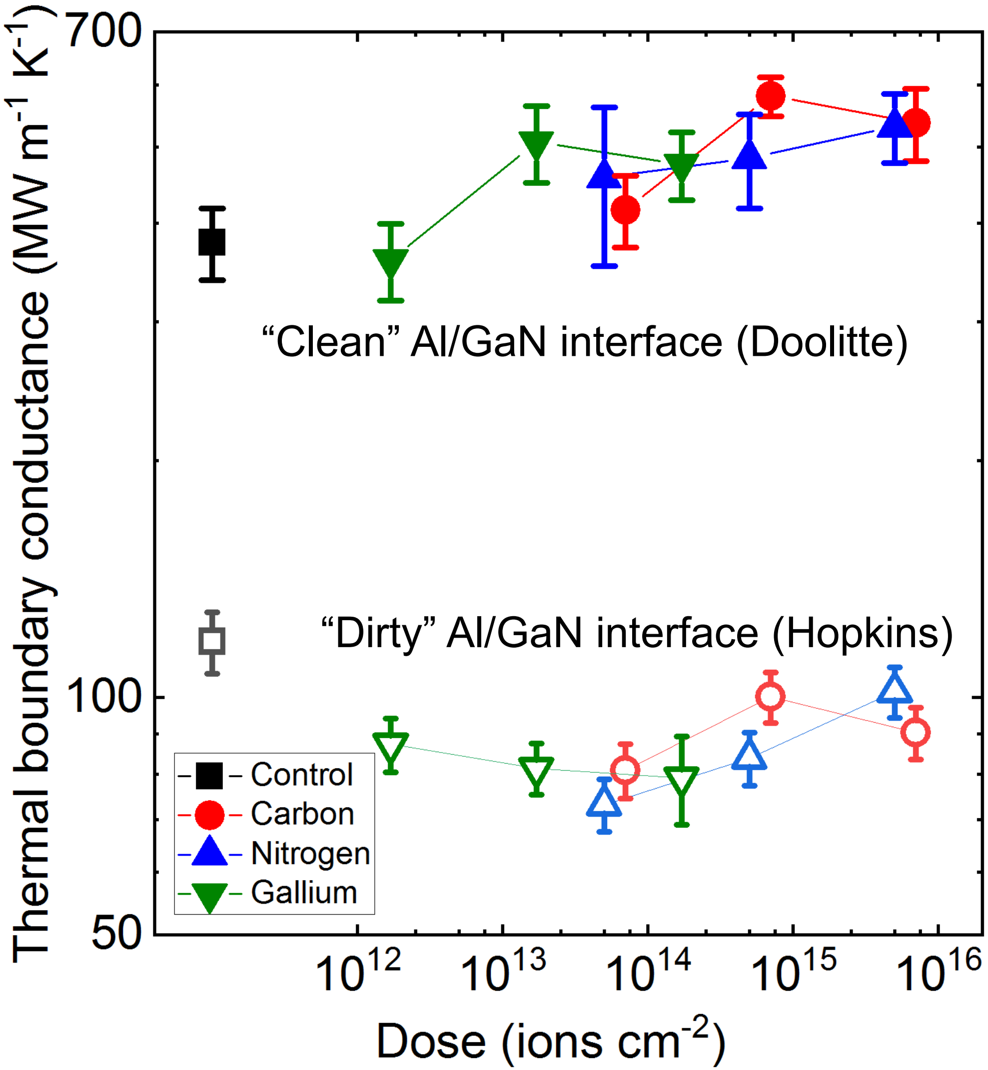
Lee and Luo, *Appl. Phys. Lett.* **112**, 011603

Ion-irradiation induced defects enhance GaN phonon TBC

And interfacial defects can control the population and density of states of these modes



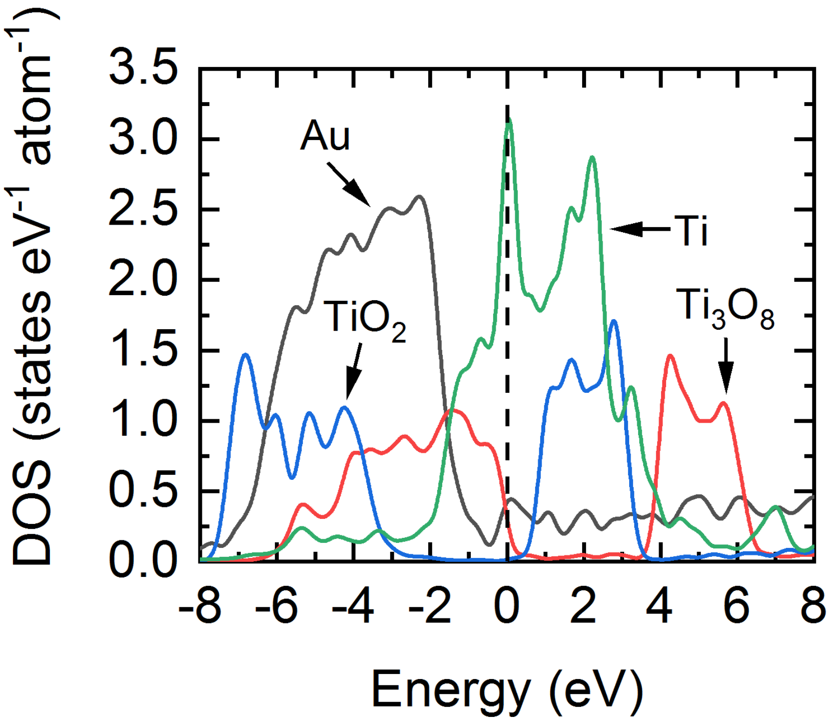
400 keV He+ implants: end of range dep

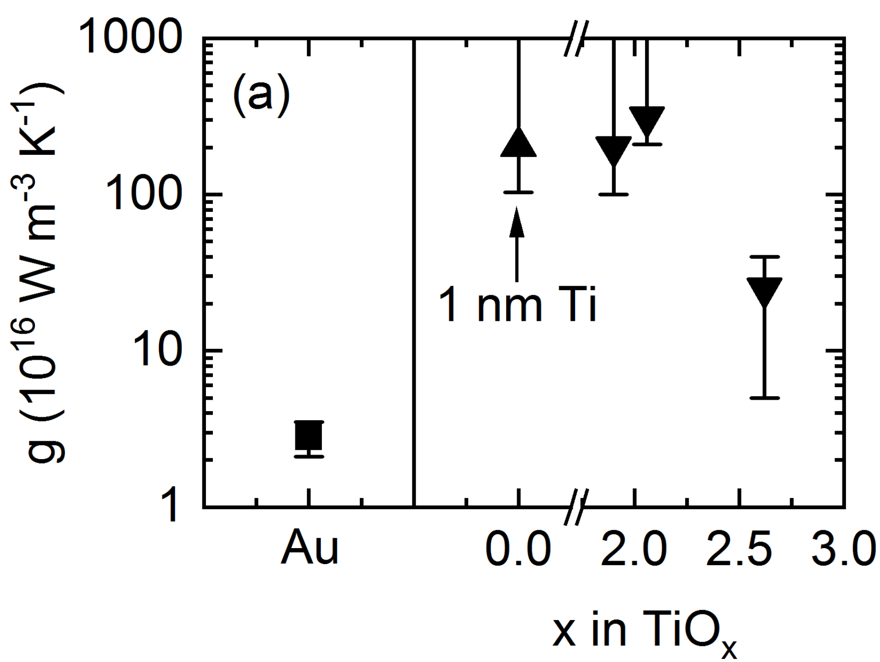


Collaboration: Khalid Hattar (SNL)

Defects enhance electron-phonon interfacial coupling

Coupled electron-phonon thermal resistance can be impact by chemistry at interfaces based on defect vibrational energies

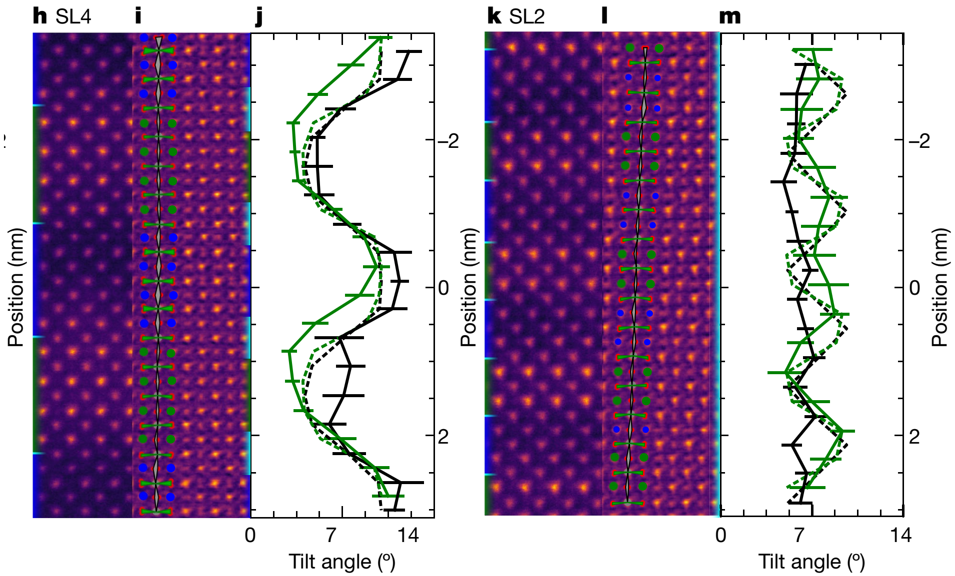


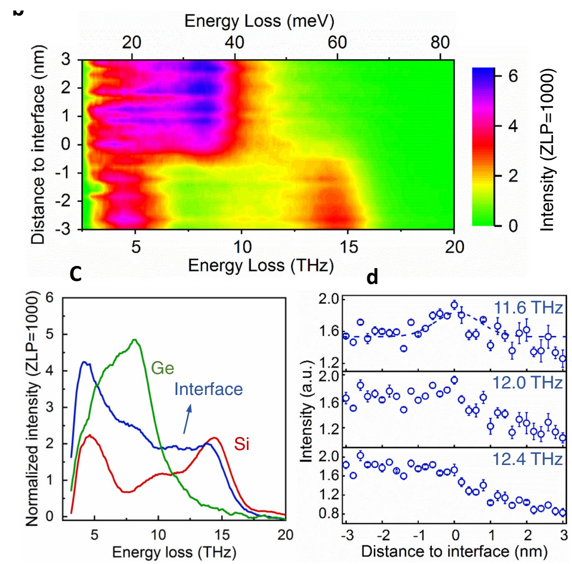


Olson *et al. Appl. Phys. Lett.* **118**, 163503

Technical challenge: spectrally resolve the existence of these unique phononic states at polar WBC and UWBG interfaces

STEM EELS offers unprecedented spatial and energy resolution to resolve these unique modes





556 | Nature | Vol 601 | 27 January 2022

NATURE COMMUNICATIONS | (2021)12:6901 |

Article

Emergent interface vibrational structure of oxide superlattices

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https://doi.org/10.1038/s41467-021-27250-3 OPEN

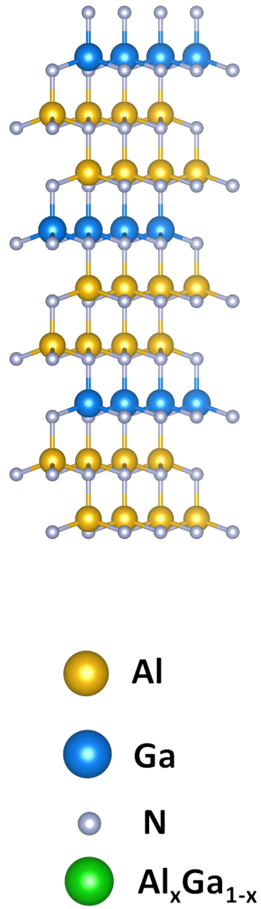
Experimental observation of localized interfacial phonon modes

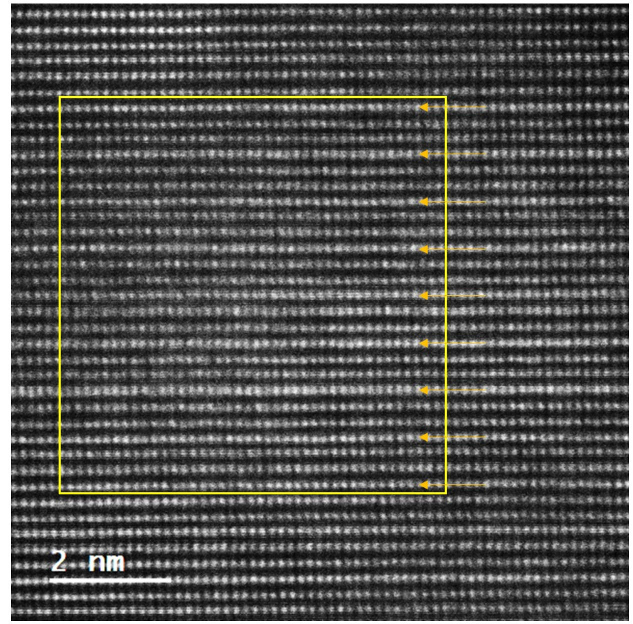
Zhe Cheng[1,10,11], Ruiyang Li[2,11], Xingxu Yan[3,4,11], Glenn Jernigan[5], Jingjing Shi[1], Michael E. Liao[6], Nicholas J. Hines[1], Chaitanya A. Gadre[7], Juan Carlos Idrobo[8], Eungkyu Lee[9], Karl D. Hobart[5], Mark S. Goorsky[6], Xiaoqing Pan[3,4,7✉], Tengfei Luo[2✉] & Samuel Graham[1✉]

Technical challenge: Engineering WBG and UWBG materials to enhance the contribution to these modes

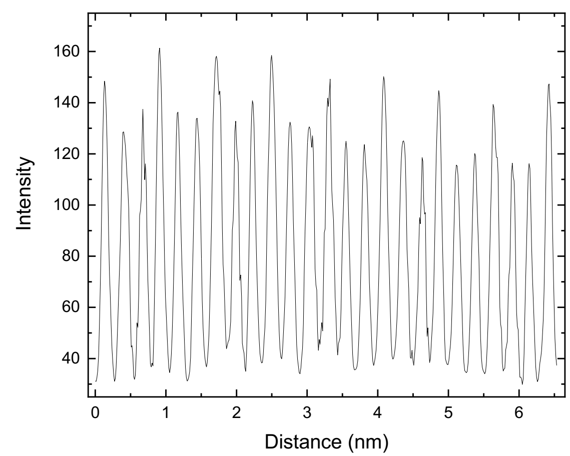
The “digital alloy” – can we chemically order “defects”?

- Digital alloys of varying periodicity grown by **Khan** and measured by **Goorsky**



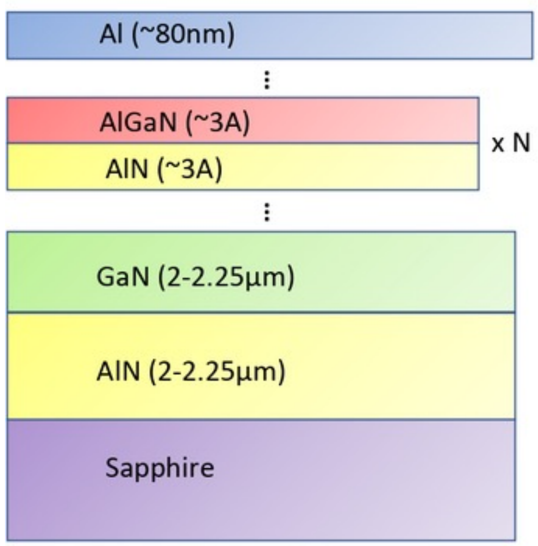


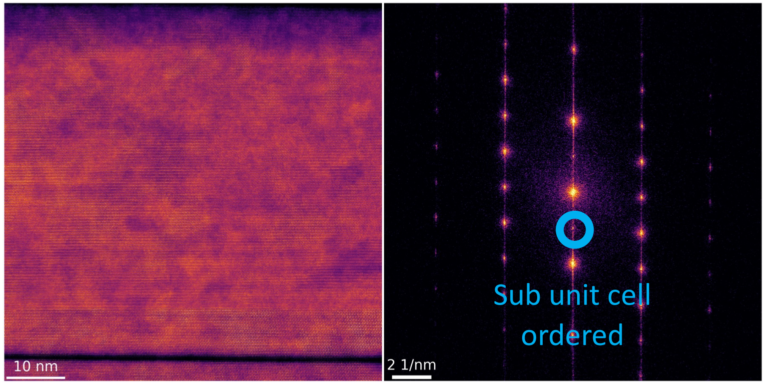
- Thickness varying from a few nanometers to ~200 nm

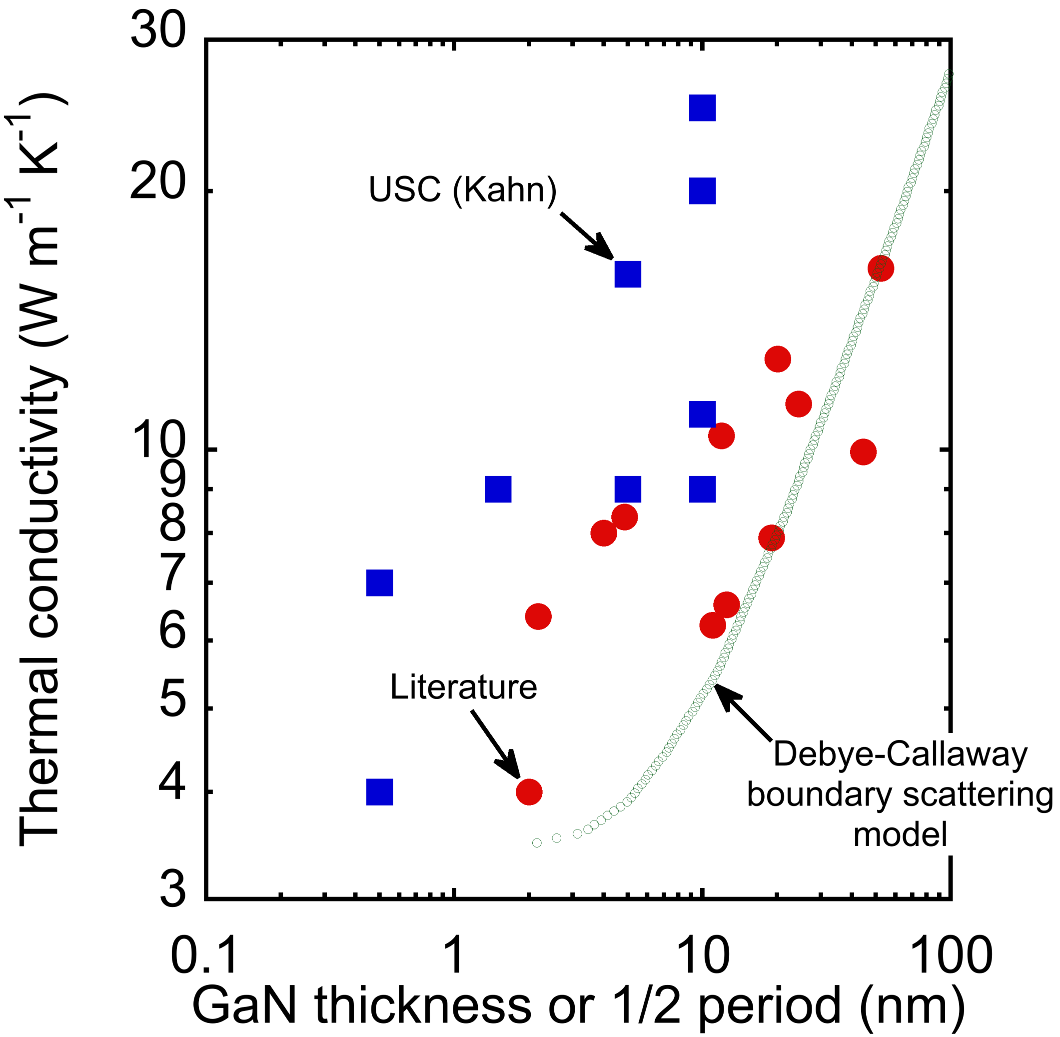


Technical challenge: Engineering WBG and UWBG materials to enhance the contribution to these modes

High quality SLs and the "digital alloy"

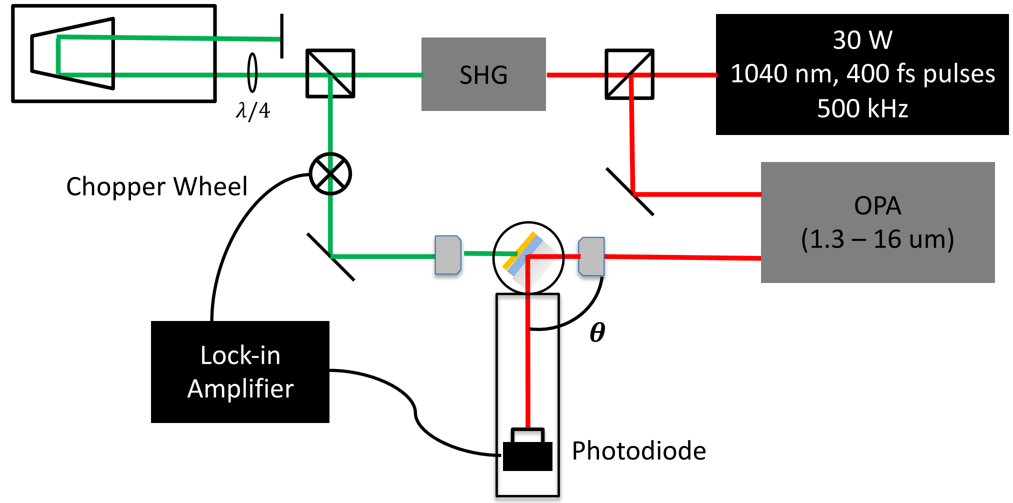


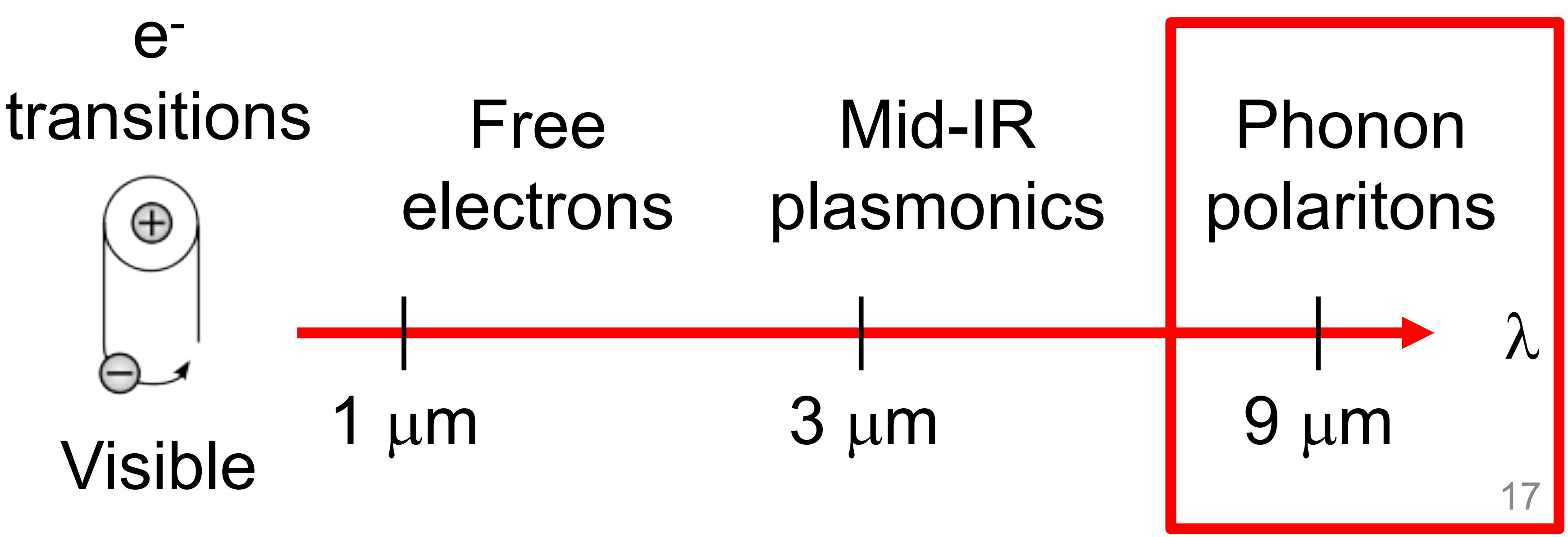




Technical challenge: spectrally resolve the contribution of these modes to thermal transport

Can we measure the contribution to thermal conductivity from individual phonon modes?





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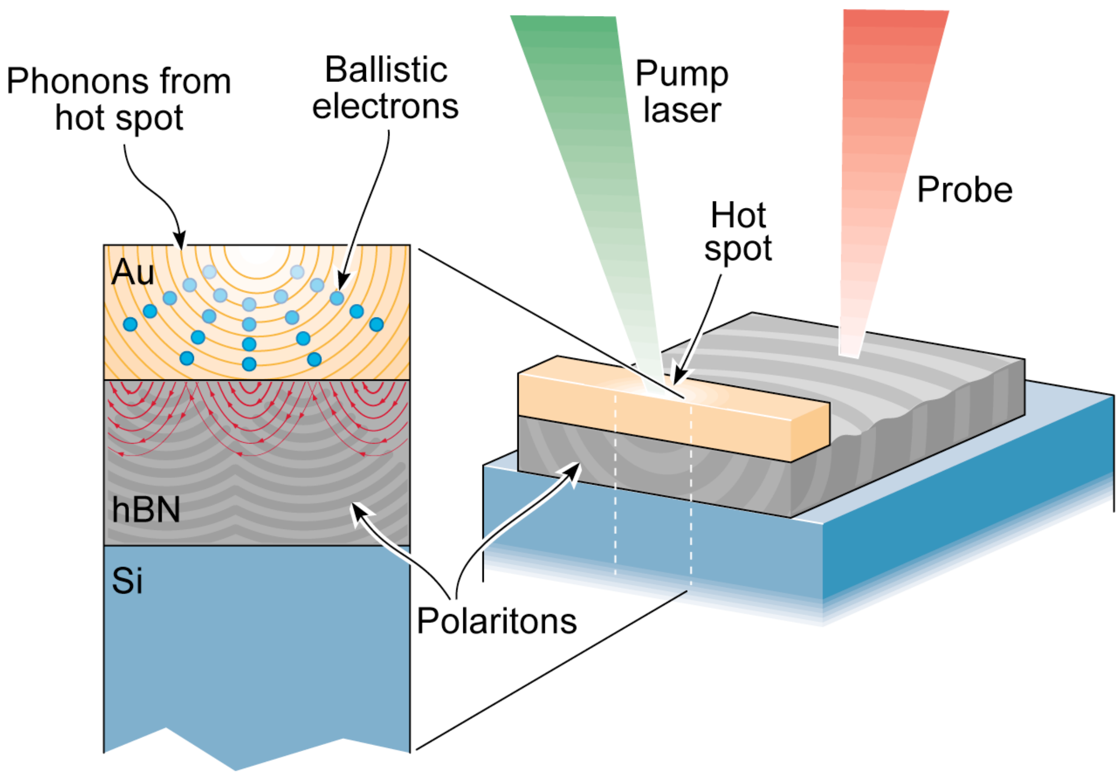


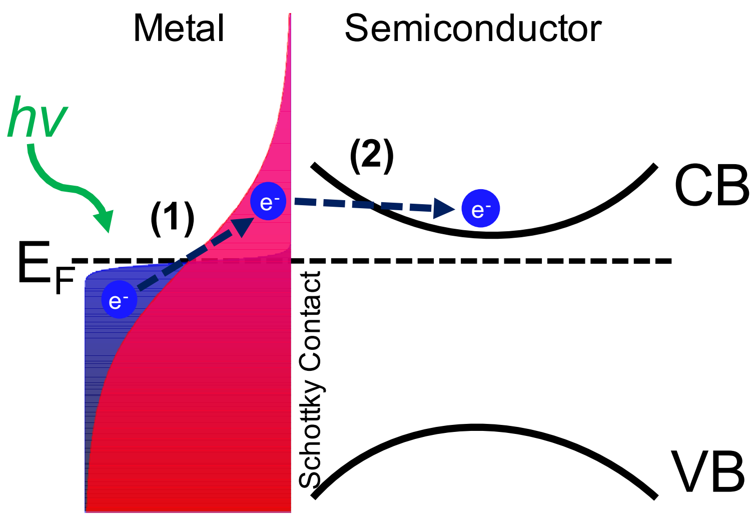
Can we measure the contribution to thermal conductivity from individual phonon modes?

Collaboration under ARO funding
Caldwell (Vanderbilt), Maria (PSU)

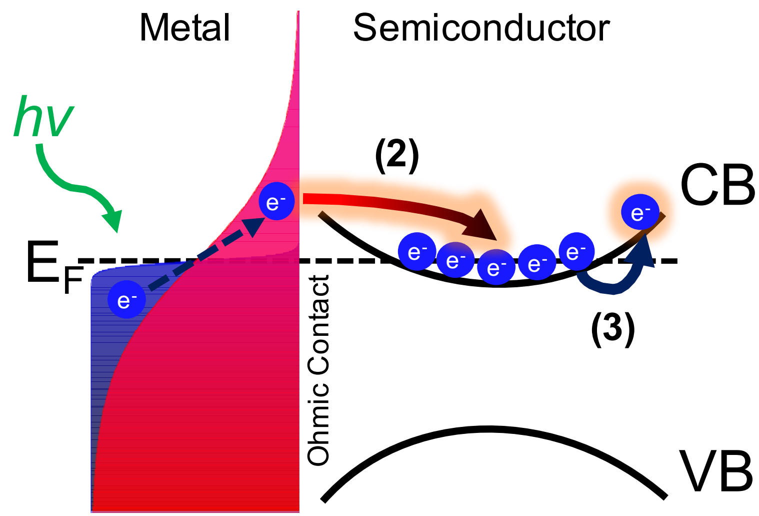
Technical challenge: Move beyond phonon engineering and enhance TBC with electronic mechanisms

Recall: electron-electron TBC is ultrahigh compared to phonon-phonon TBC: how can we embrace this for UWBG material cooling?

a) Hot electron injection (Charge transfer)



b) Ballistic thermal injection (Energy transfer)



Tomko *et al. Nature Nano.* **16**, 47
Collaboration under ARO funding
Caldwell (Vanderbilt), Maria (PSU), Prezhdo (USC)

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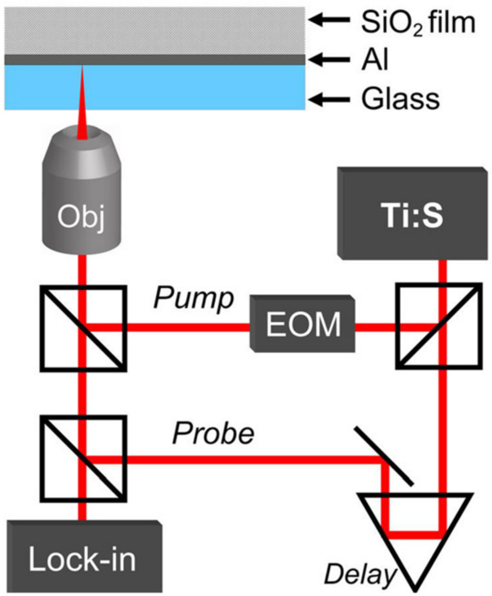
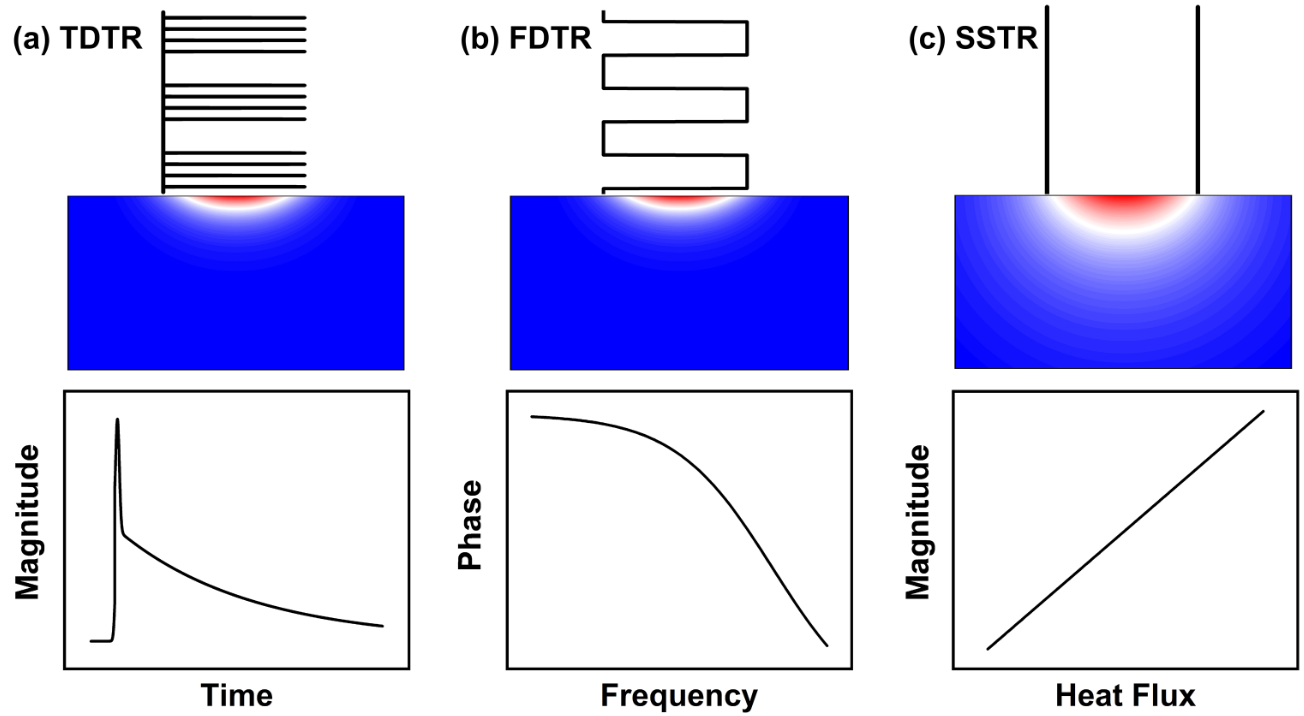
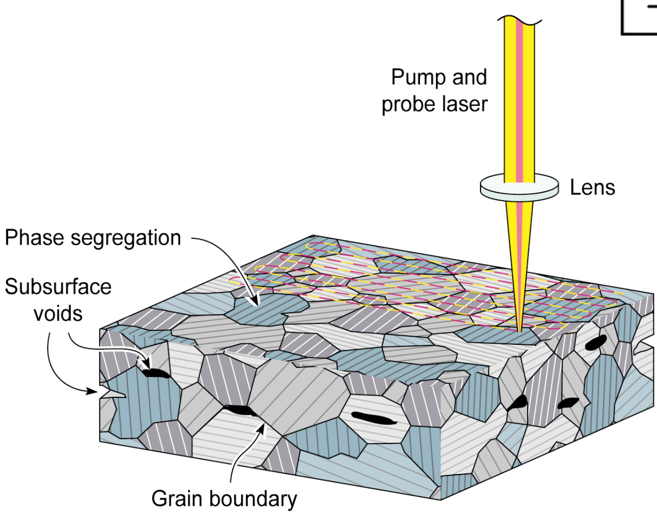
But how do we measure nano to macro HX processes?







Spatially resolved thermoreflectance techniques for thermal conductivity measurements from the nanoscale to the mesoscale

Cite as: J. Appl. Phys. **126**, 150901 (2019); doi: 10.1063/1.5120310
Submitted: 17 July 2019 · Accepted: 29 September 2019 ·
Published Online: 16 October 2019

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David H. Olson,[1] Jeffrey L. Braun,[1] and Patrick E. Hopkins[1,2,3,a)]

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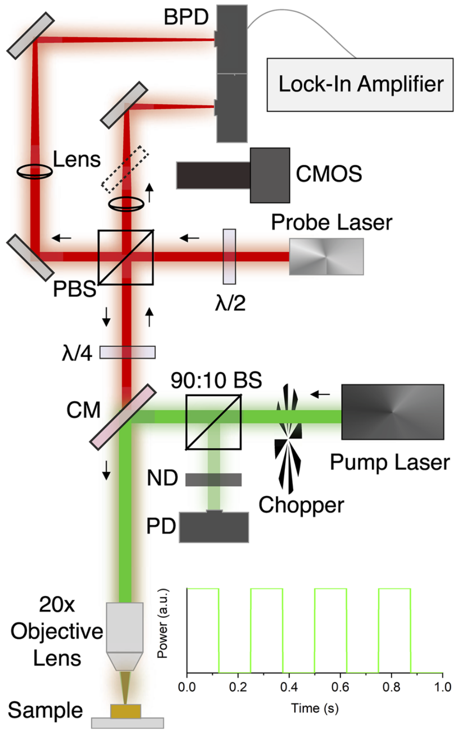

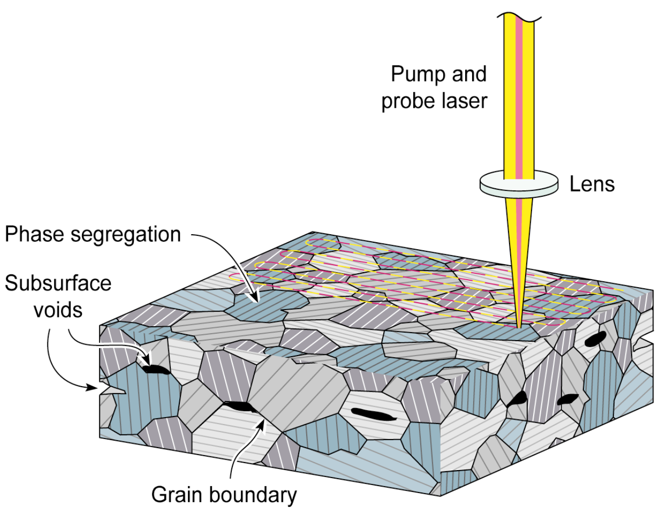

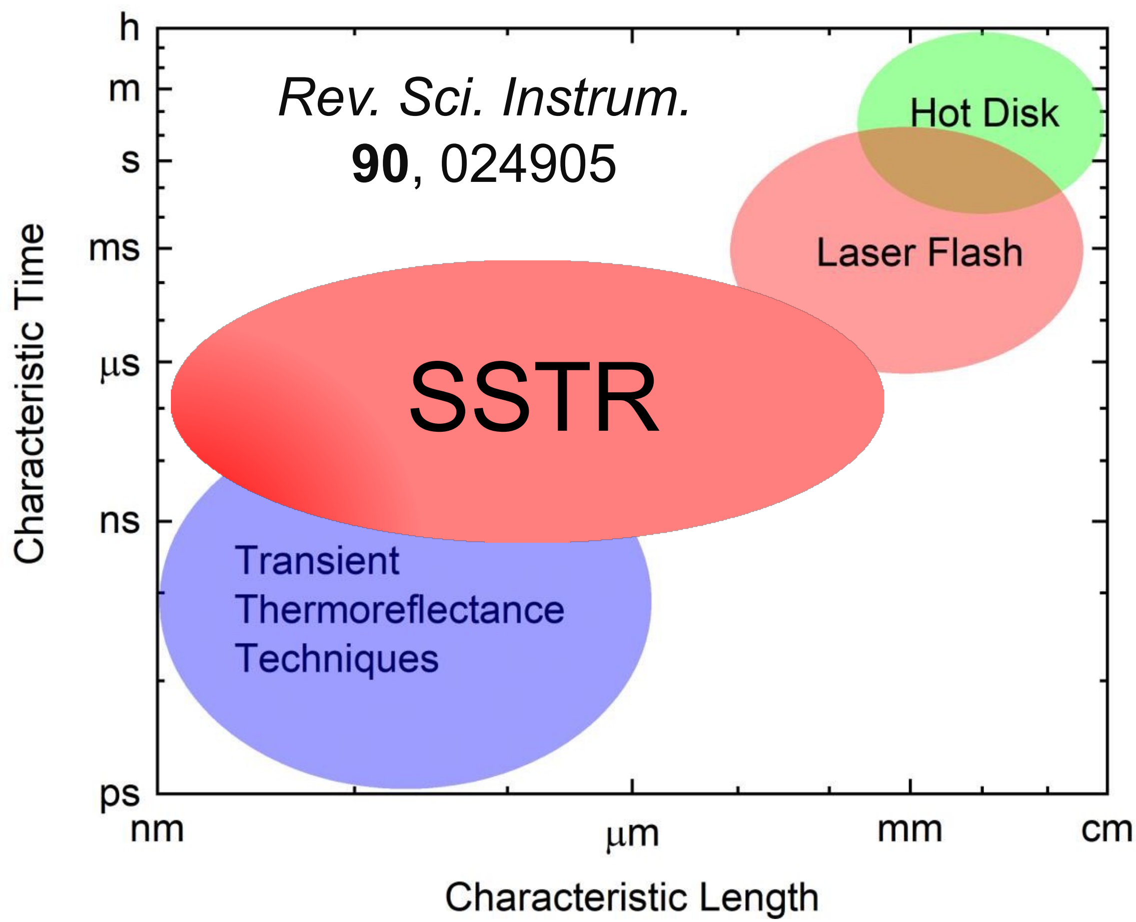

Spatially resolved thermoreflectance techniques for thermal conductivity measurements from the nanoscale to the mesoscale EP

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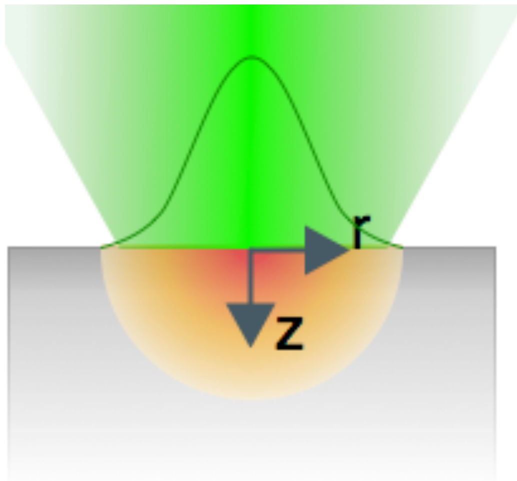
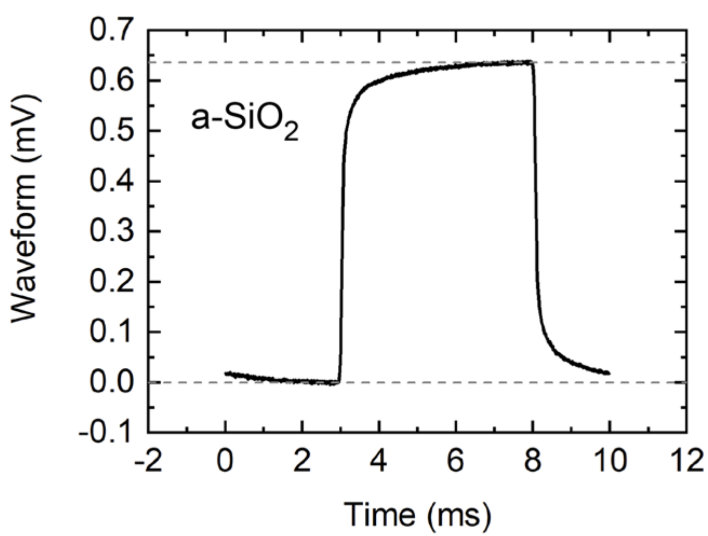
Submitted: 17 July 2019 · Accepted: 29 September 2019 ·
Published Online: 16 October 2019

David H. Olson,[1] Jeffrey L. Braun,[1] and Patrick E. Hopkins[1,2,3,a)]

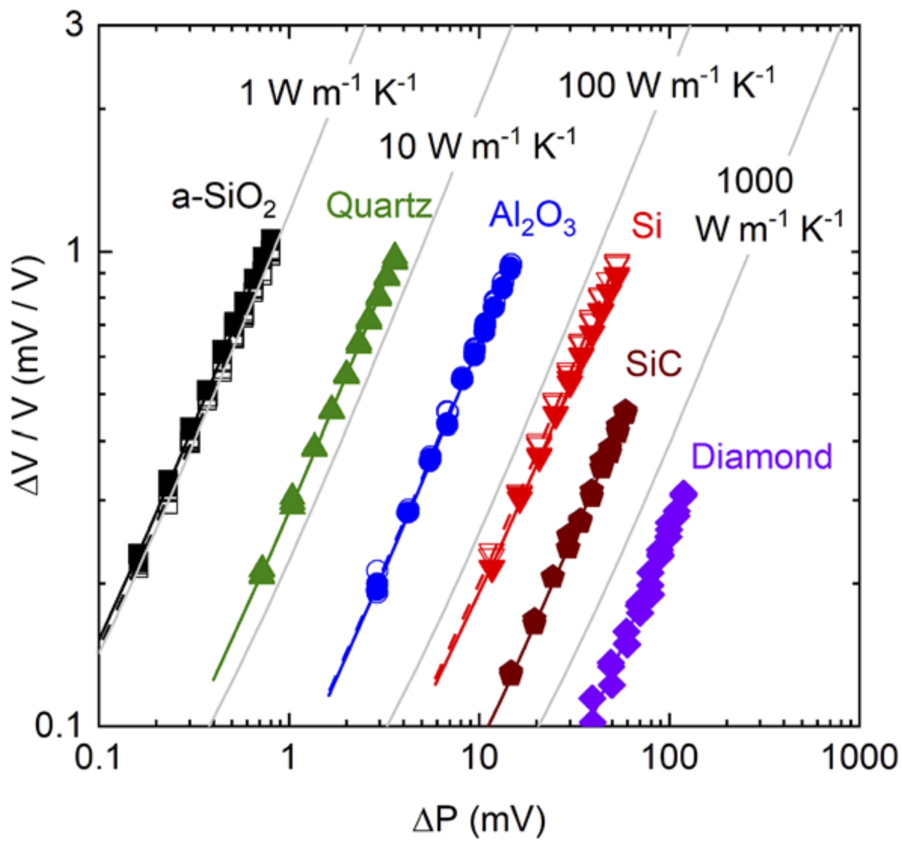
Steady-state thermoreflectance (SSTR): How does it work?





$$Q = -k\nabla T$$

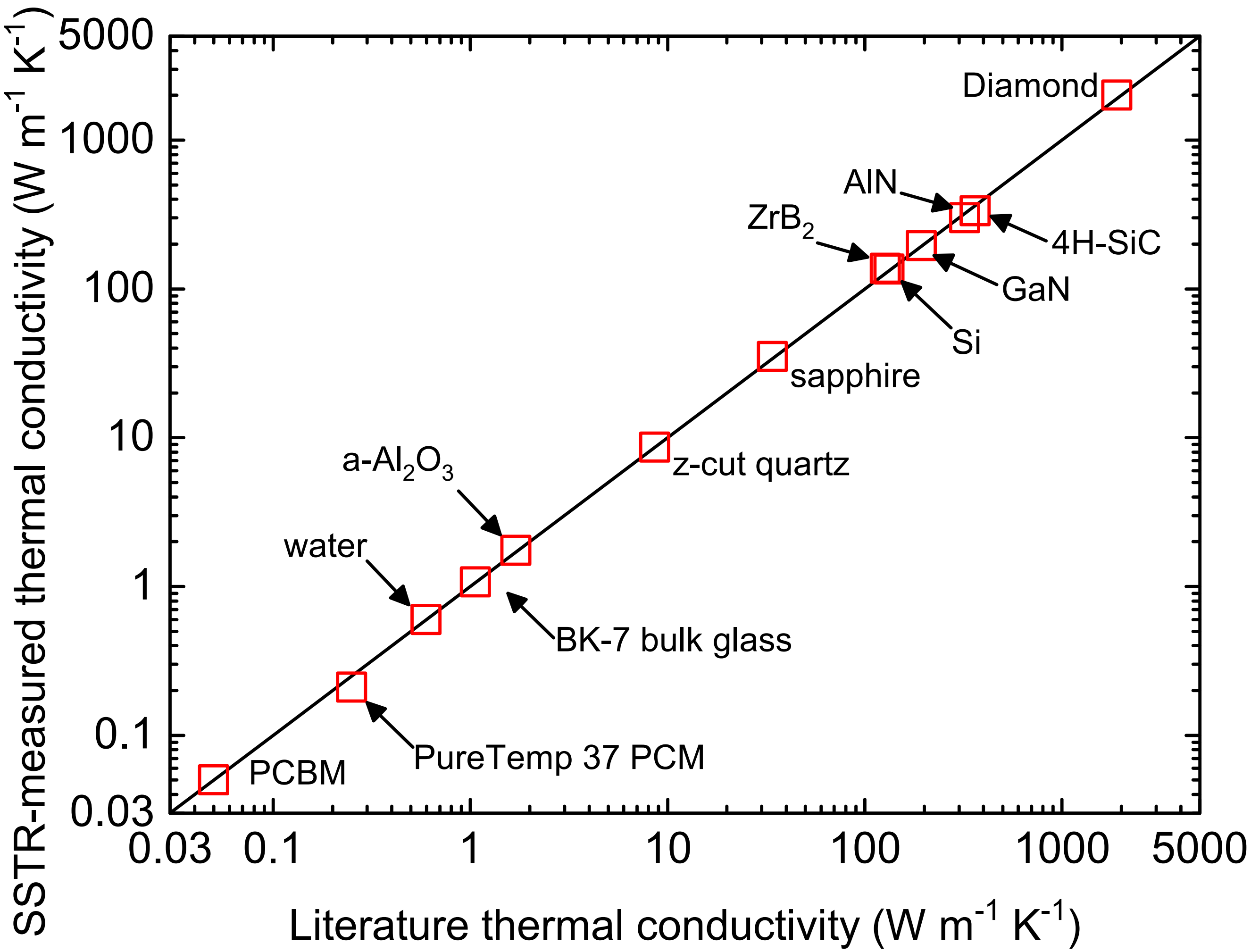
Fourier's Law



Rev. Sci. Intrum. **90**, 024905 (2019)

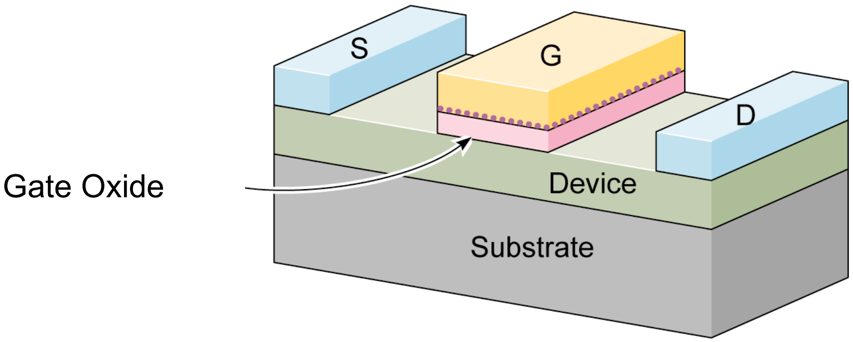
SSTR: Capabilities for thermal conductivity measurements

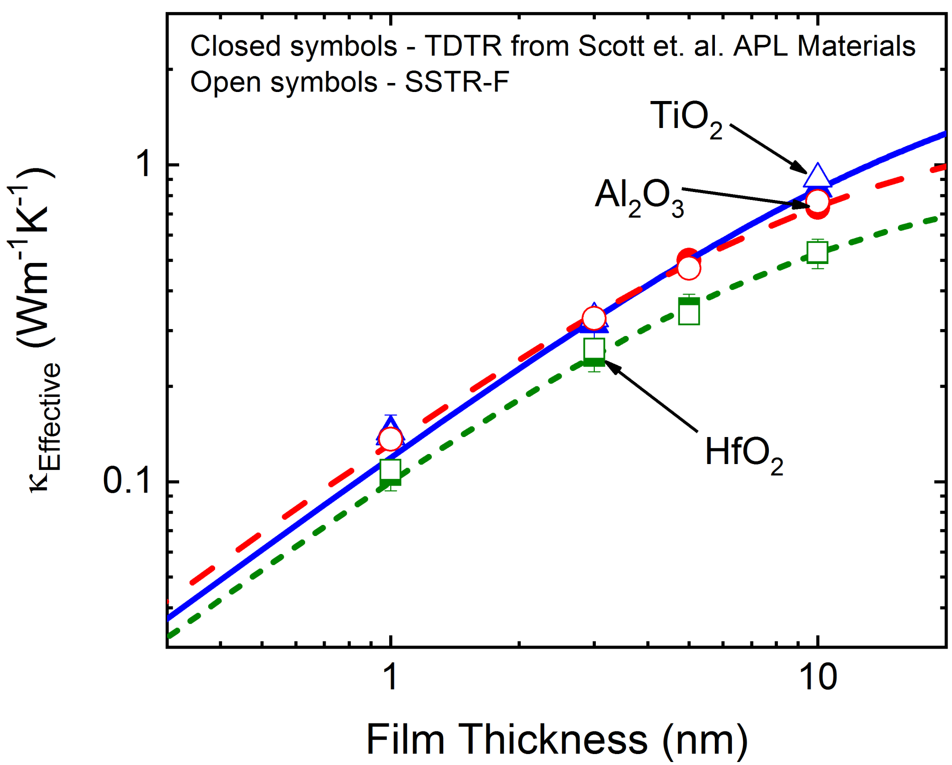
Extremely conductive (diamond) and insulative (PCBM) materials



SSTR: Capabilities for thermal conductivity measurements

Thermal conductivity of dielectric films as thin as 1 nm

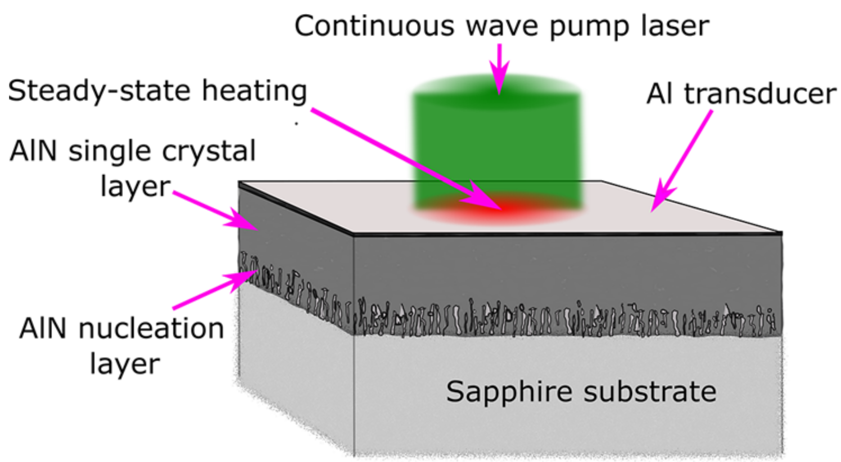


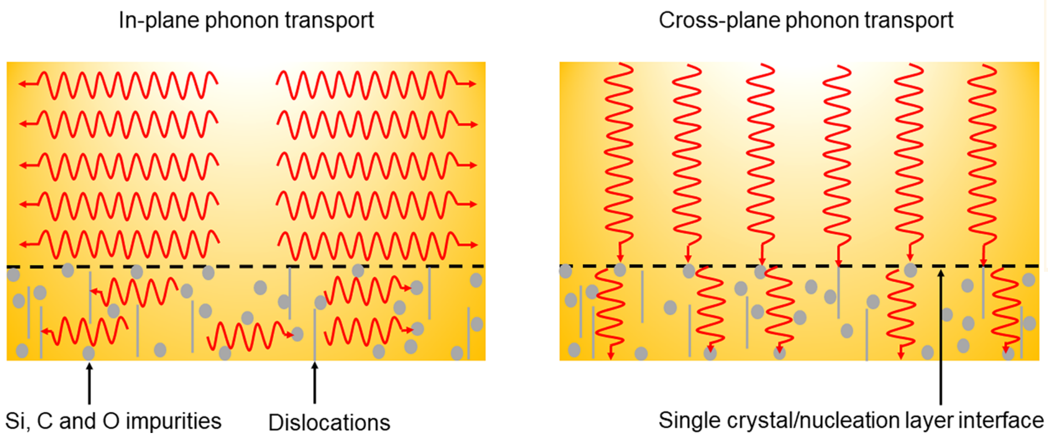


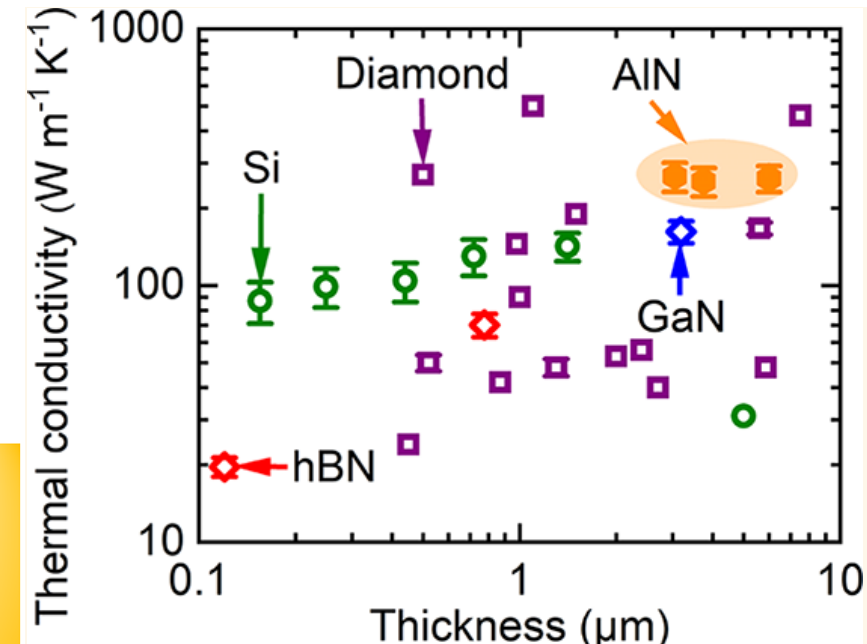
- Verified over three materials systems using SSTR-F
- Matches existing TDTR measurements
- Measuring resistance from interfaces and from material resistance in this case

APL Materials **6**, 058302 (2018)

In-plane thermal conductivity of thin films i.e., anisotropy effects in AlN thin films



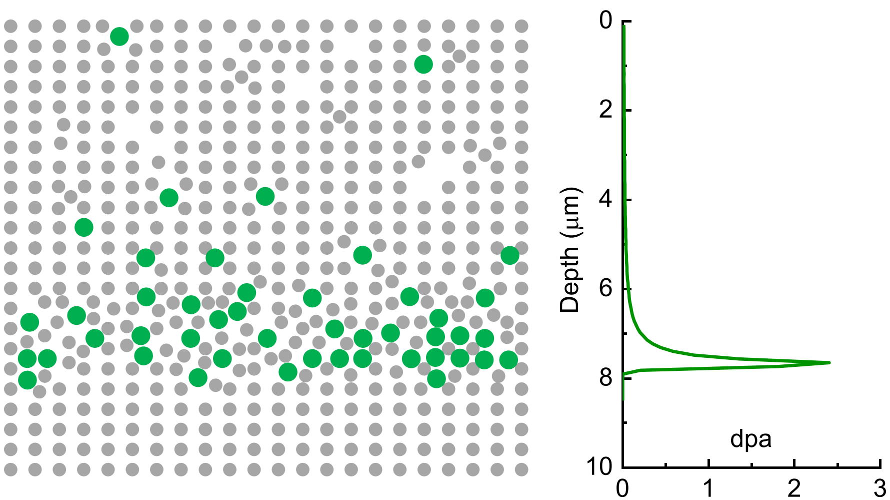


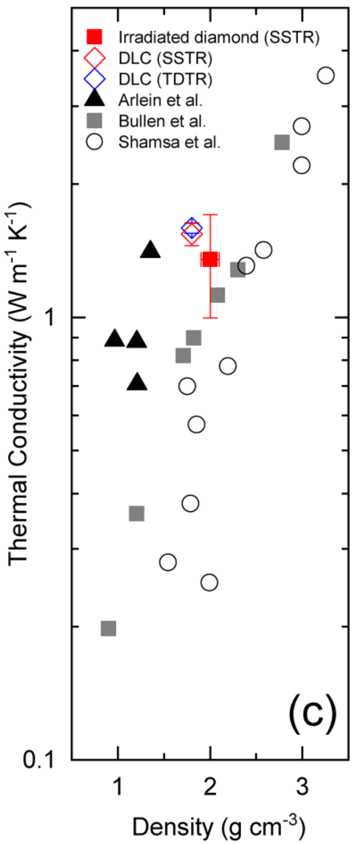


ACS Nano **15**, 9588

SSTR: Capabilities for thermal conductivity measurements

Sub-surface defect detection
(e.g., measure thermal conductivity of thin region with point defects 7 μm under diamond surface)

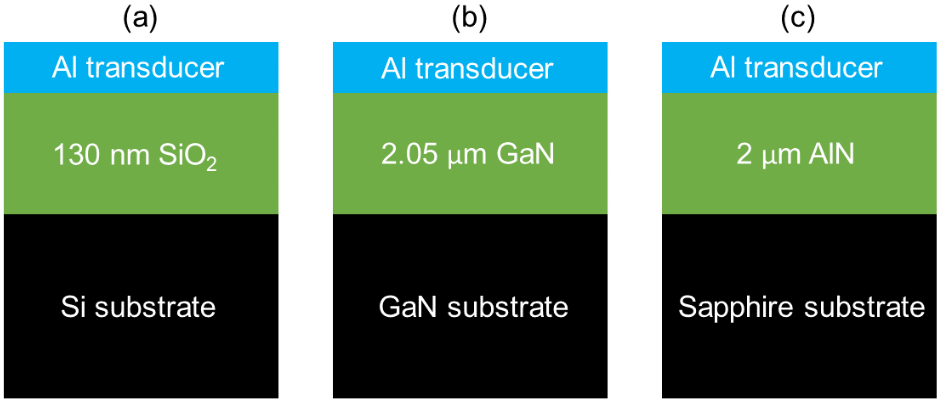




J. Appl. Phys. **15**, 9588

SSTR: Capabilities for thermal conductivity measurements

Sub-surface interfaces and heat sinks
e.g., measure thermal conductivity of buried interfaces, sub-mounts & substrates under GaN and AlN thin films



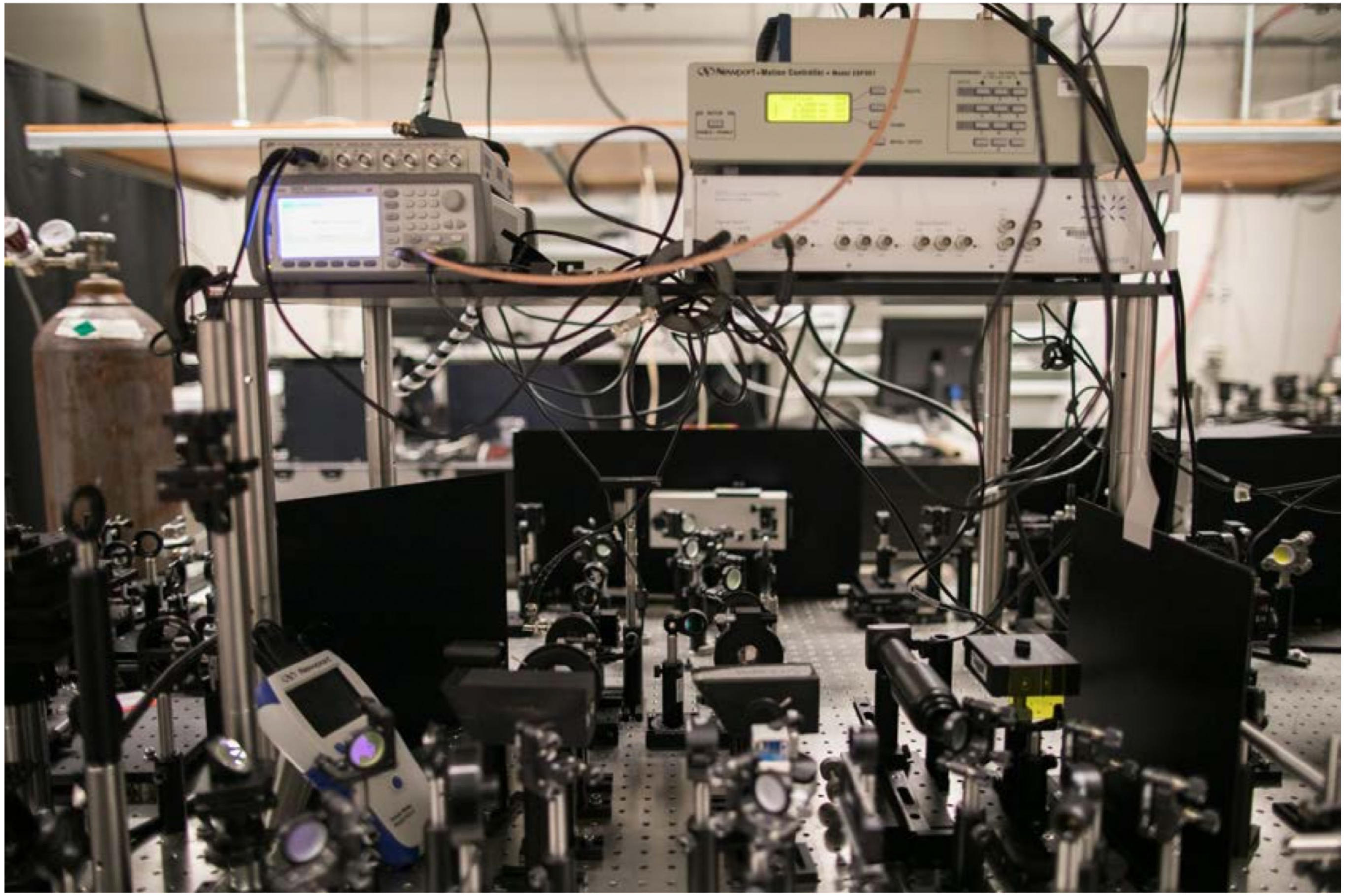
- Automated variable spot size in SSTR-F allow for control over sample depth
- Measurement of layer-by-layer thermal conductivity in electronic device stack

Substrates	Thermal conductivity ($W\ m^{-1}\ K^{-1}$)		
	spot size 10 μm	spot size 20 μm	literature
Si	141 ± 27	140 ± 18	140[30]
GaN	194 ± 27	185 ± 16	195[41]
Sapphire	35.1 ± 5.9	34.5 ± 4.2	35[42]

Rev. Sci. Intrum. **92**, 064906

SSTR-F: Recently commercialized for turn-key, fiber-optically integrated thermal conductivity microscope

The typical thermoreflectance set up

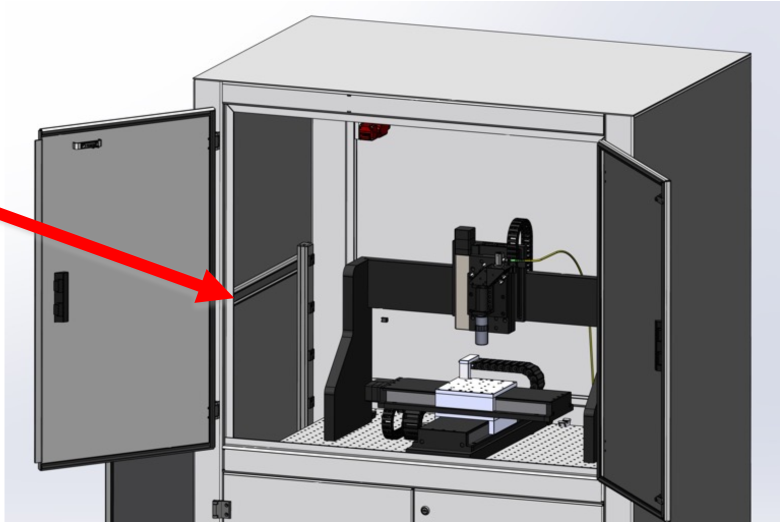


A LOT of optics, upkeep and expertise for analysis

SSTR-F: Commercialized for turn-key thermal conductivity microscope for bulk materials, thin films and interfaces

https://Laserthermal.com

LASER THERMAL



FULL DISCLOSURE: HOPKINS IS A CO-FOUNDER OF THIS COMPANY

Summary and key challenges

- Key Take Away #1: Defects and interfaces can be developed to **enhance** electron and phonon thermal transport
  - *Challenge*: Growth of thin films with controlled spatial arrangements of defects and interfaces
  - *Challenge*: Harness coupled carriers (e.g., electron-phonon, polaritons) to bypass large phonon transport and directionally control thermal transport

- Key Take Away #2: New metrologies can measure spatial, temporal and spectral contribution of electron and phonon transport
  - *Challenge*: Measure and manipulate interfacial modes to enhance thermal transport
  - *Challenge*: Measure and manipulate coupled carrier's contribution to thermal transport across interface
  - *Challenge*: Translate thermal metrologies to materials and device labs and industry