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Thermal boundary conductance across heteroepitaxially grown ZnO/GaN interfaces

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NANO LETTERS

Letter

Cite This: *Nano Lett.* 2018, 18, 7469–7477

pubs.acs.org/NanoLett

Thermal Boundary Conductance Across Heteroepitaxial ZnO/GaN Interfaces: Assessment of the Phonon Gas Model

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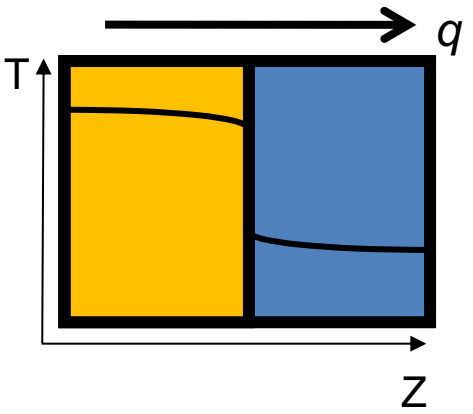
UVA

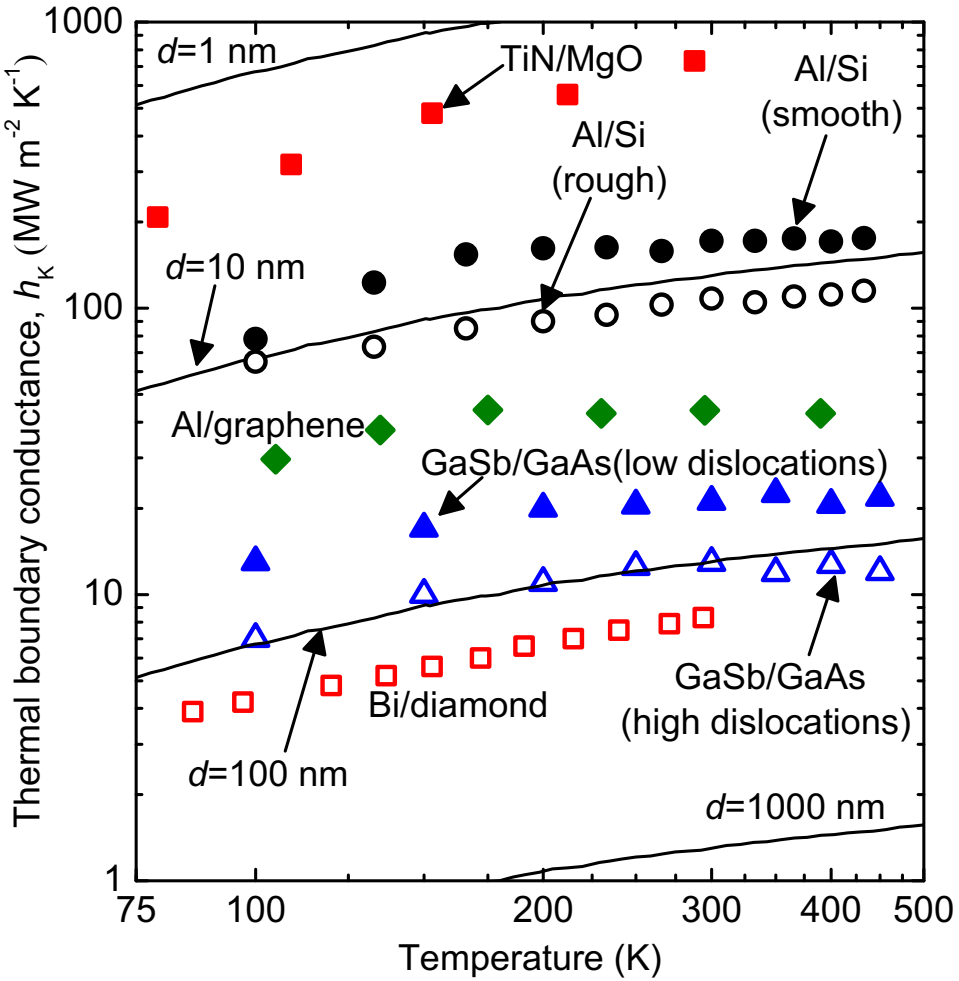
Office of Naval Research

Science & Technology

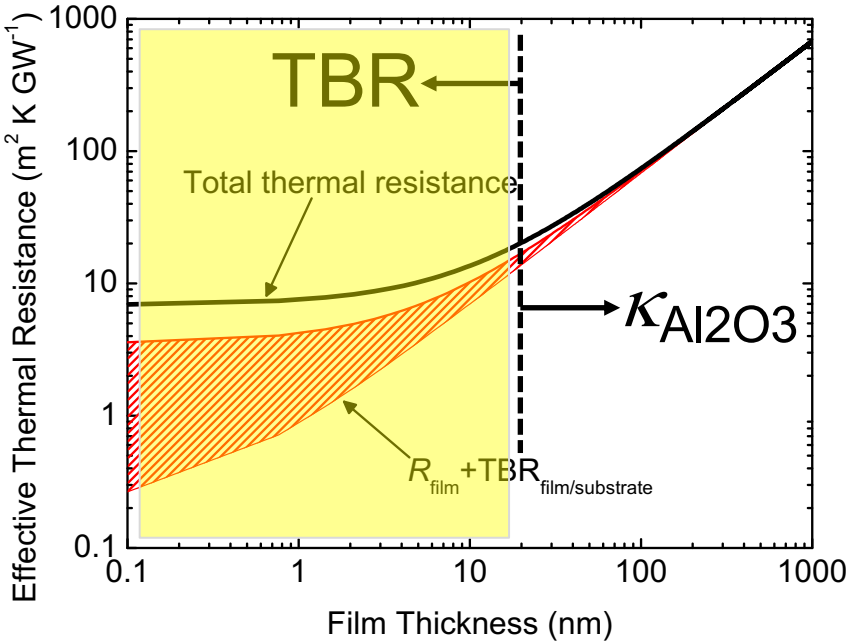
Thermal boundary conductance – nanoscale resistances

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





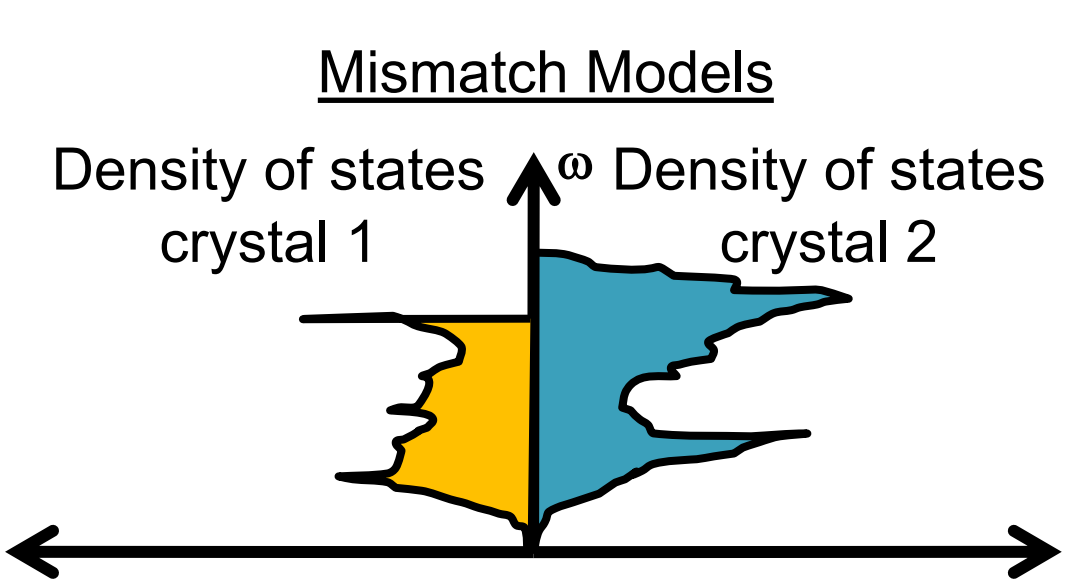
Ex: Al/ALD Al_2O_3/Si

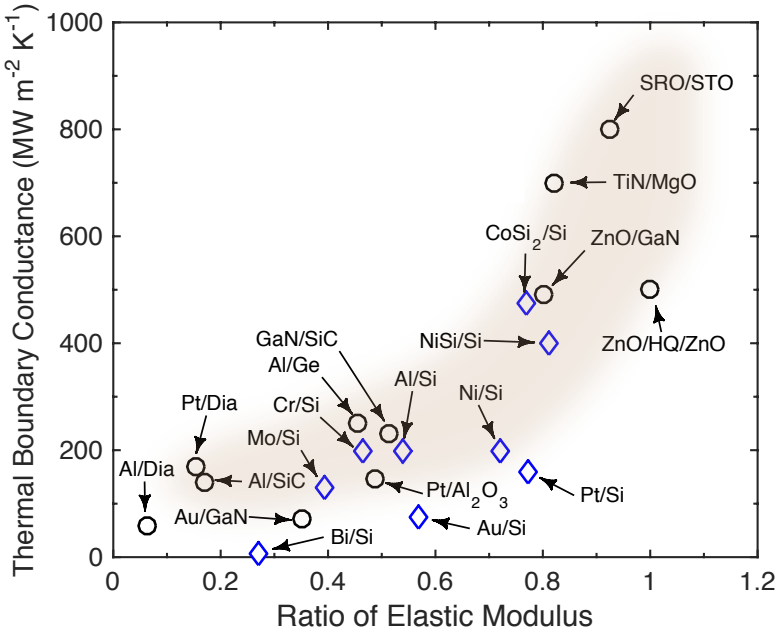


Scott *et al. APL Materials* **6**, 058302 (2018)

The basic *traditional* concept: phonon spectrum matching

$$h_K \propto \int_\omega C_\omega v_\omega \zeta_\omega \, d\omega \propto \int_\omega \hbar\omega D_\omega \frac{\partial f_\omega}{\partial T} v_\omega \zeta_\omega \, d\omega$$

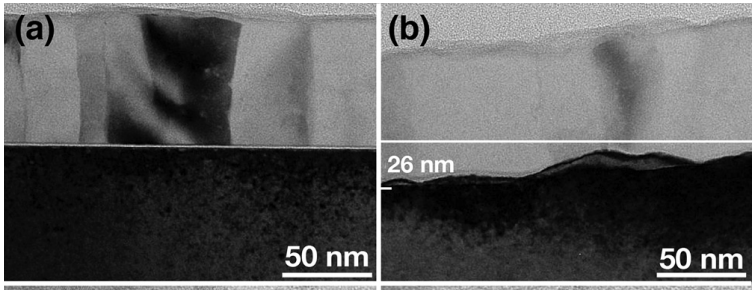


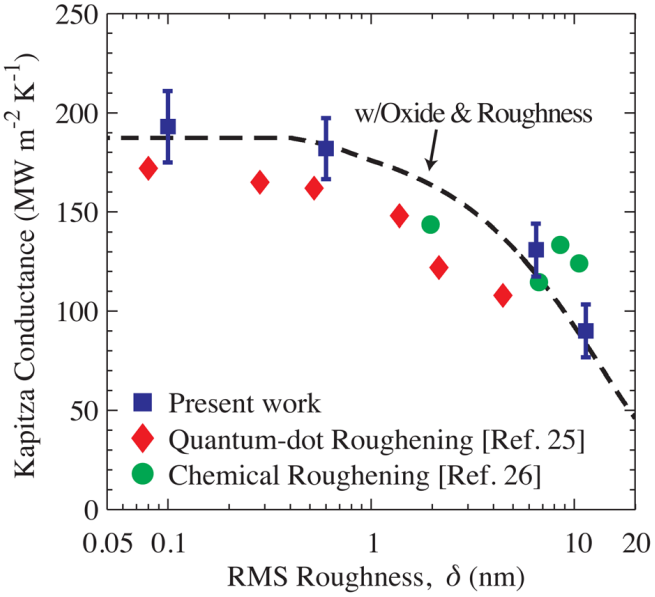


Need “high quality” crystalline interfaces to compare to/validate/verify theoretical concepts

Interfacial imperfections can change in intrinsic TBC

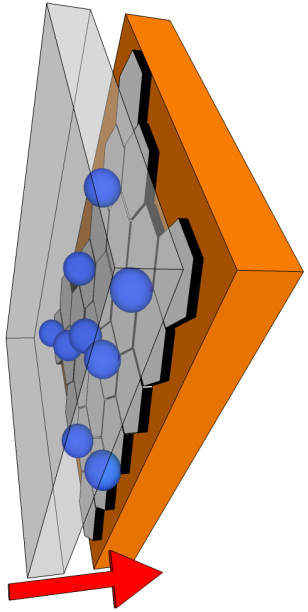
Ex: Al/Si – roughness and native oxide

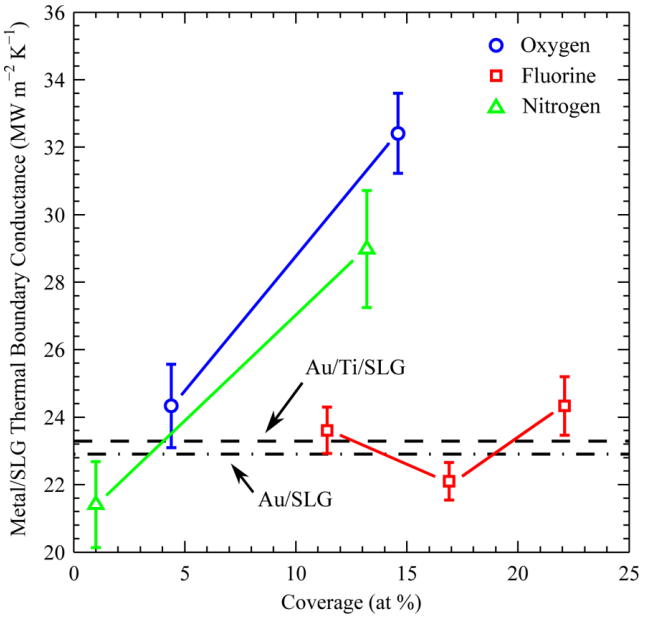




Duda & Hopkins, *Appl. Phys. Lett.* **100**, 111602 (2012)

Ex: metal/graphene – chemical functionalization





Hopkins *et al.*, *Nano Lett.* **12**, 590 (2012)
Foley *et al.*, *Nano Lett.* **15**, 4876 (2015)
Walton *et al.*, *Surf. & Coat. Tech.* **314**, 148 (2017)

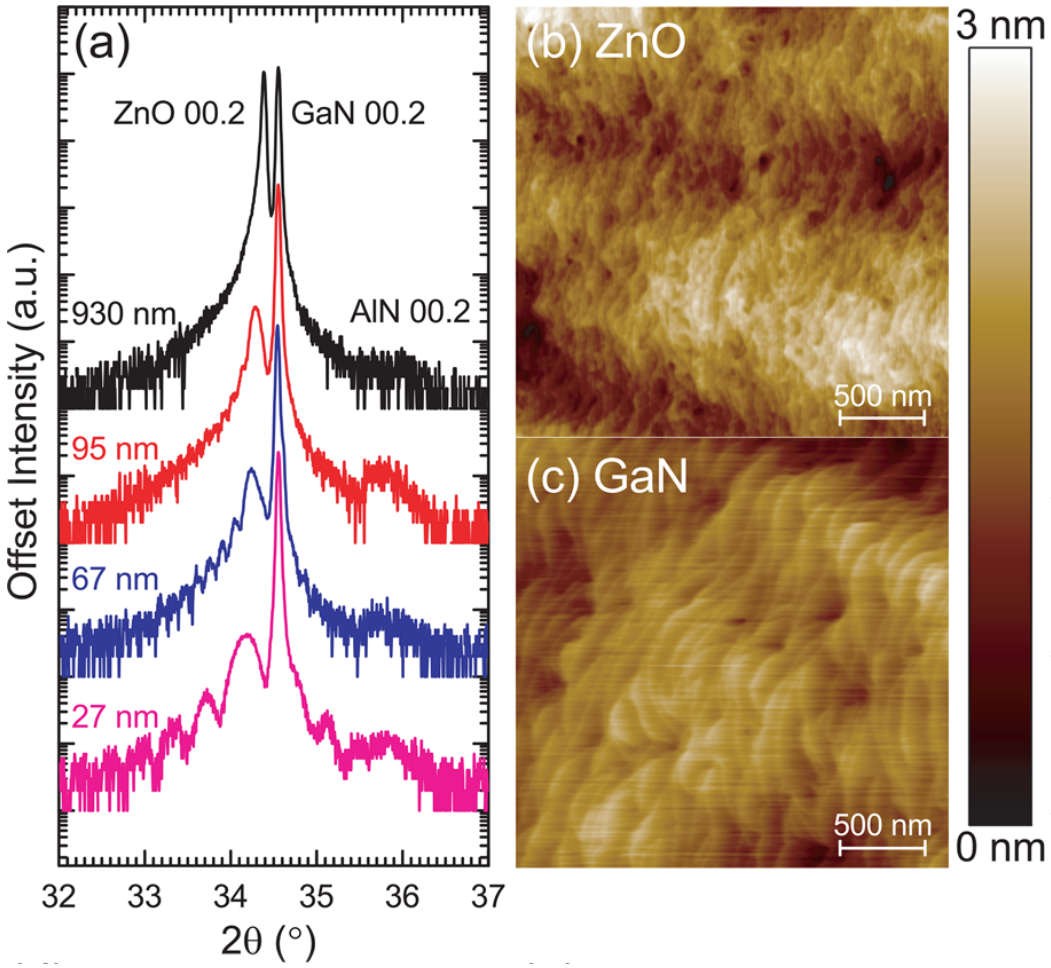
Previous work on "epitaxial" interfaces – and our study

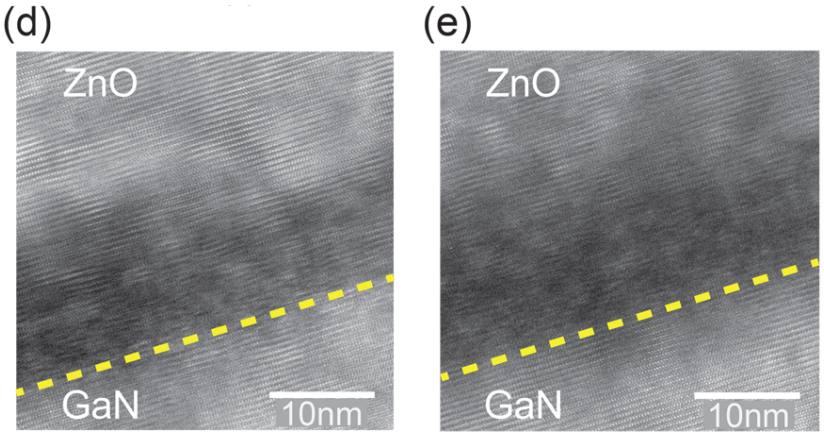
- Need "high quality" crystalline interfaces to compare to/validate/verify theoretical concepts
- Previous "epitaxial" interfaces are metal/non-metal
  - Ex: Bi/Si (Horn-von Hoegen)
  - Ex: TiN/MgO (Cahill)
  - Ex: $SrRuO_3/SrTiO_3$ (Cahill)
  - Ex: Silicide/Si (Feser, Fisher, Janotti)

- Our Goal: Use TDTR to measure TBC across heteroepitaxially grown ZnO on GaN substrates
- *Nearly* ideal interface to study in tandem with theoretical models (DMM, AGF)
- Gaskins *et al*. *Nano Letters* **18**, 7469 (2018)

Heteroepitaxial ZnO on Gan/Sapphire

Growth by G. Kotsonis and JP Maria (PSU)

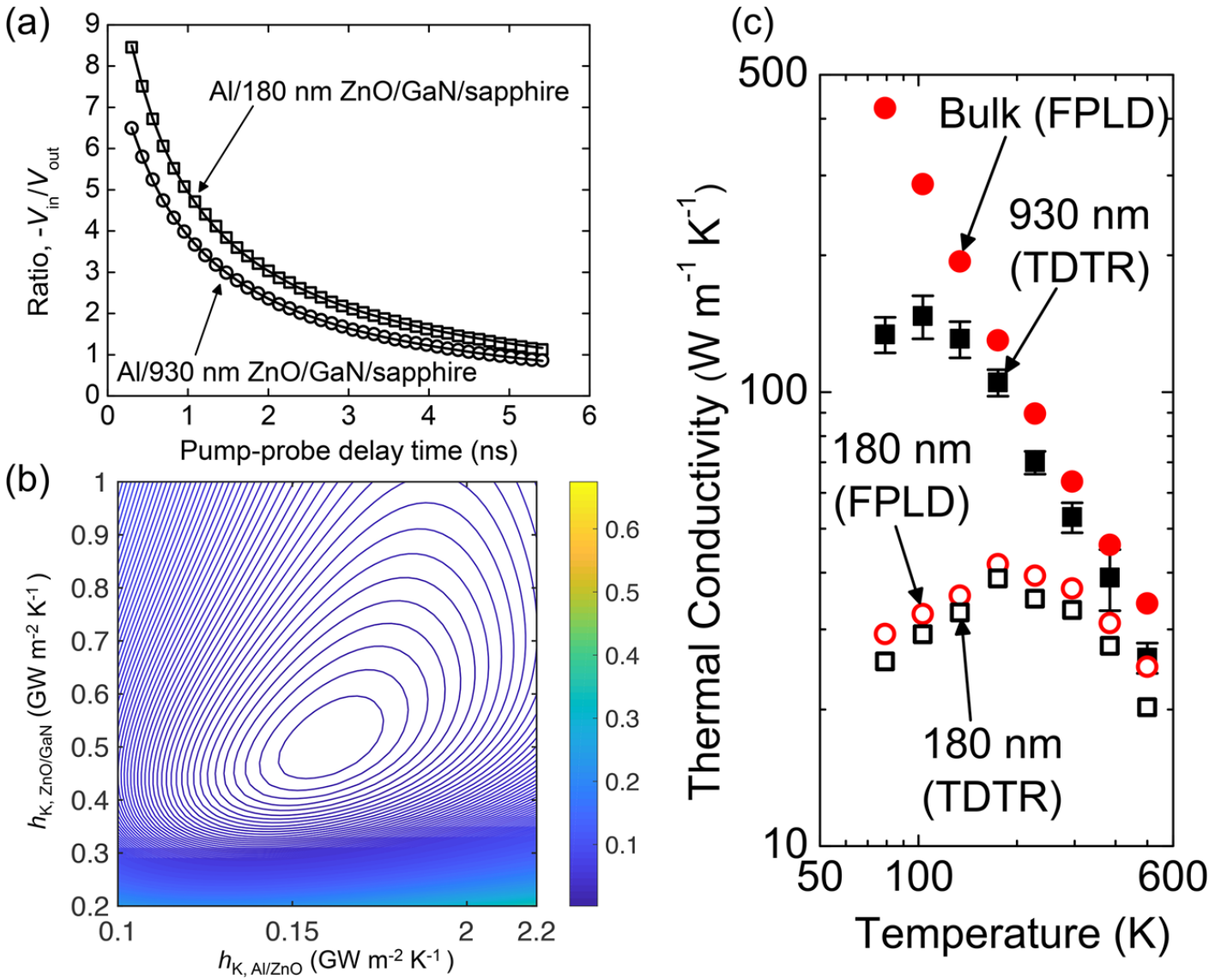




- Thermal conductivity ZnO:
  d_{ZnO} = 930 nm
- TBC ZnO/GaN:
  d_{ZnO} = 95, 180 nm
- Resistance check of Al/ZnO/GaN:
  d_{ZnO} = 5,10,19,27,42,66 nm

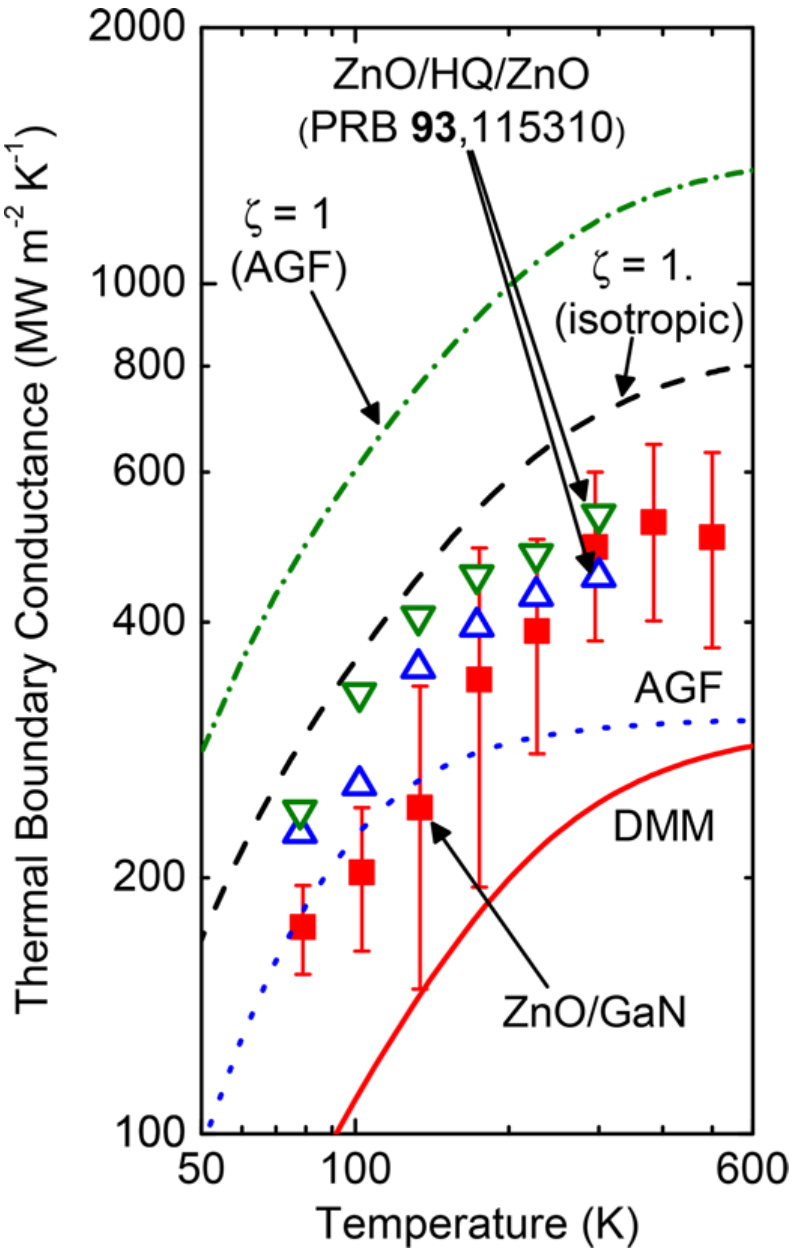
Gaskins *et al*. *Nano Letters* **18**, 7469 (2018)

TDTR measurements – uncertainty and layer properties

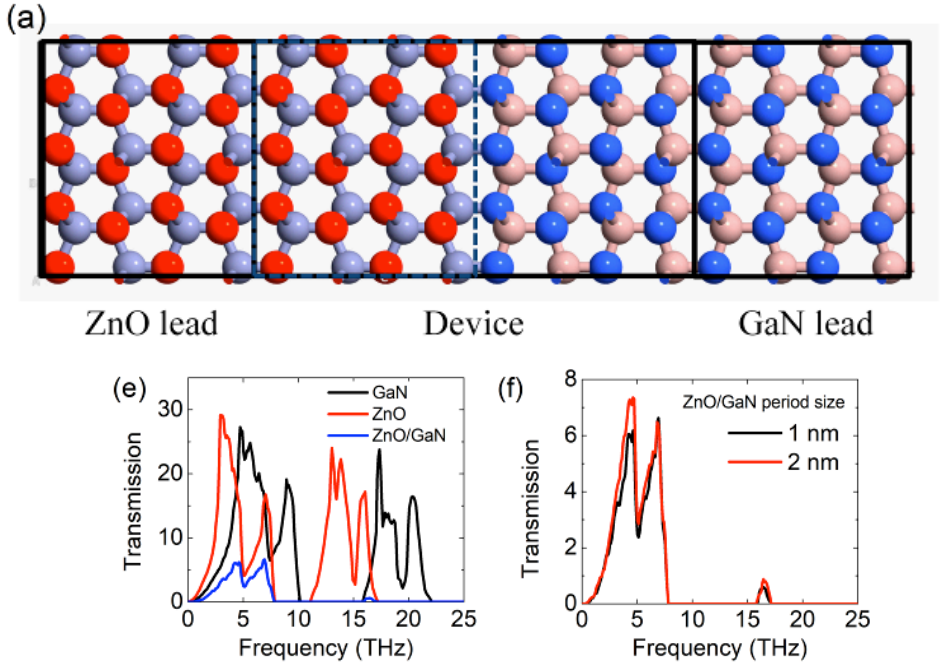


Gaskins *et al*. *Nano Letters* **18**, 7469 (2018)

TBC across ZnO/GaN interfaces

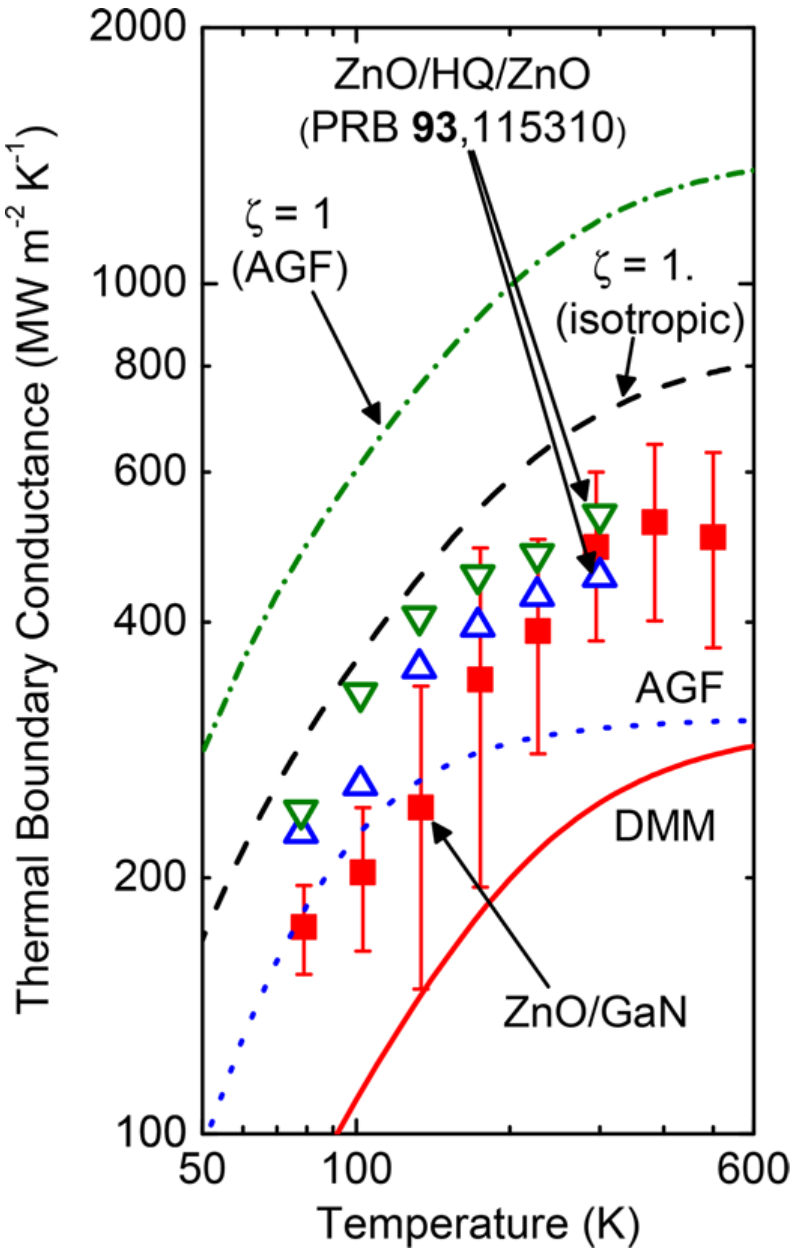


Elastic DMM and AGF can not capture high temperature TBC measurements (calcs from J. Shiomi and A. Henry)

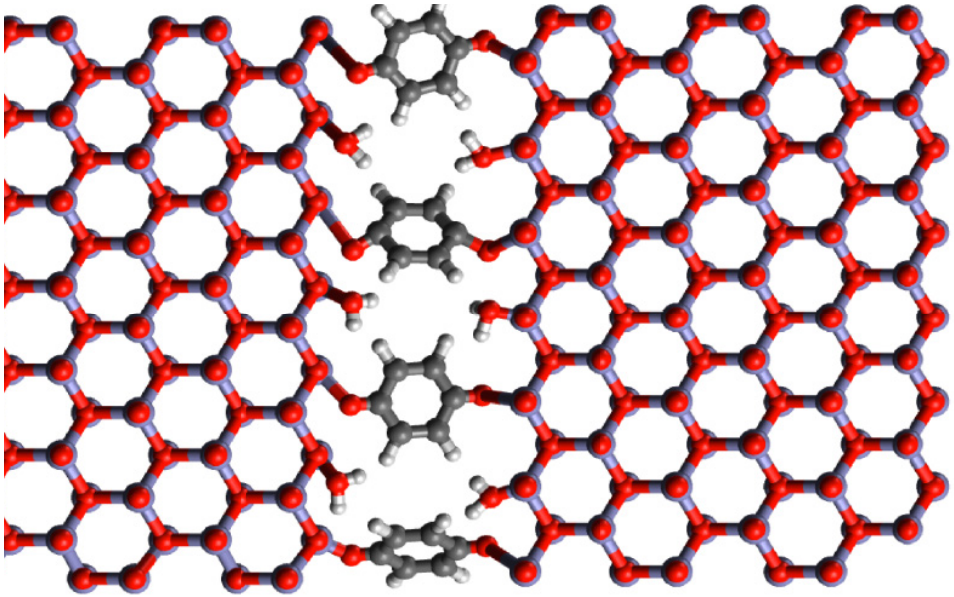


Gaskins *et al*. *Nano Letters* **18**, 7469 (2018)

TBC across ZnO/GaN interfaces

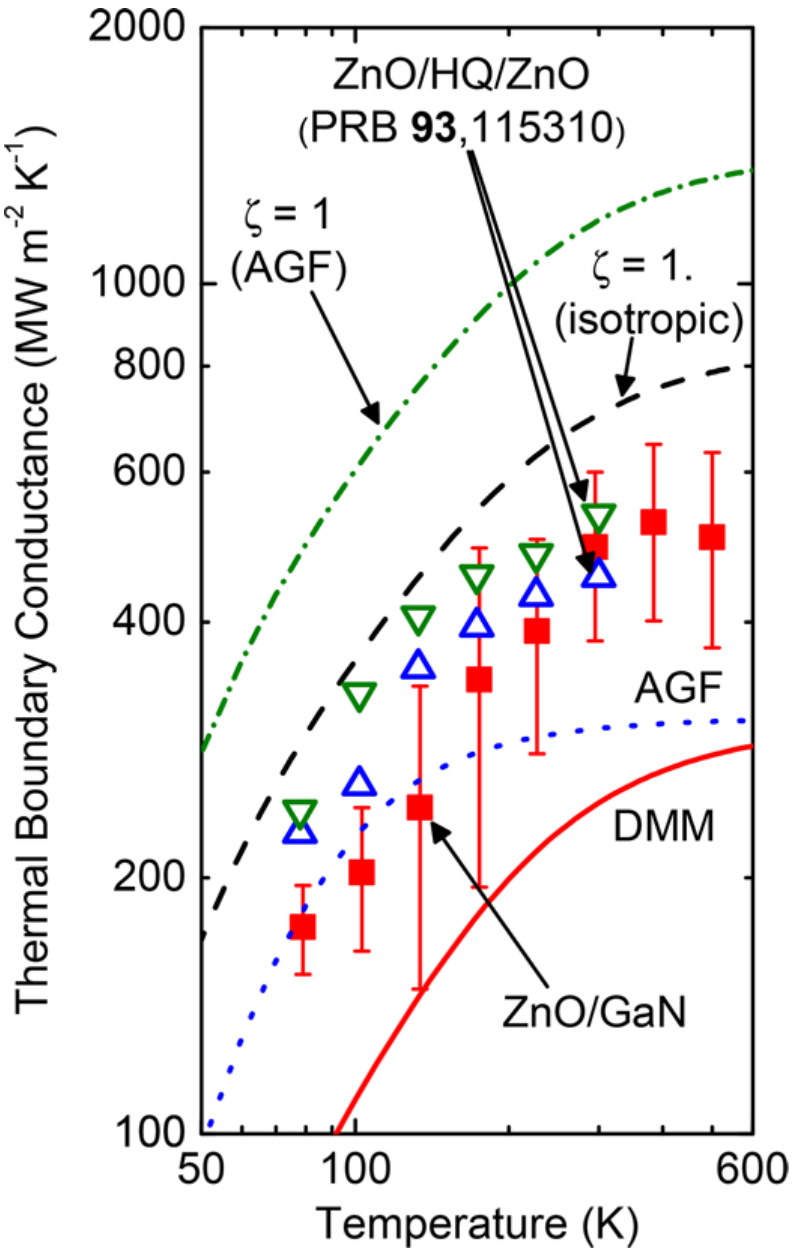


ZnO/GaN TBC similar to ZnO/HQ/ZnO TBC demonstrating upper limit to diffusive scattering

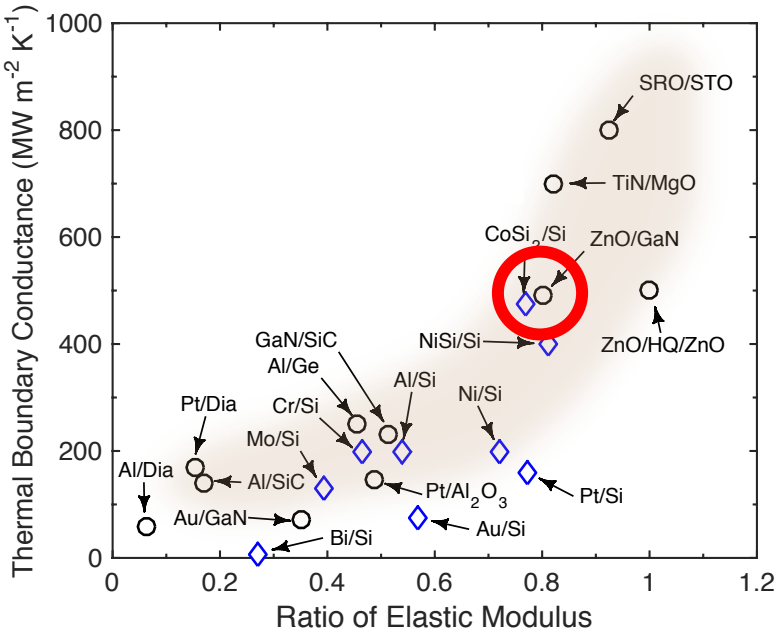


Gaskins *et al*. *Nano Letters* **18**, 7469 (2018)

TBC across ZnO/GaN interfaces



ZnO/GaN TBC highest TBC for crystalline/crystalline non-metal/non-metal to date

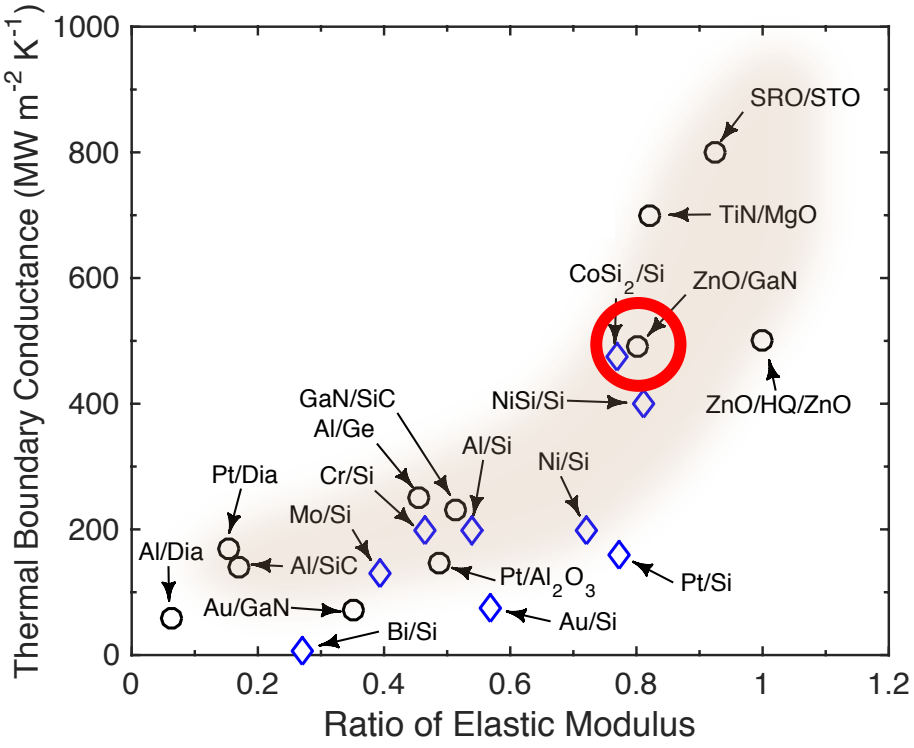


Gaskins *et al*. *Nano Letters* **18**, 7469 (2018)

Conclusions

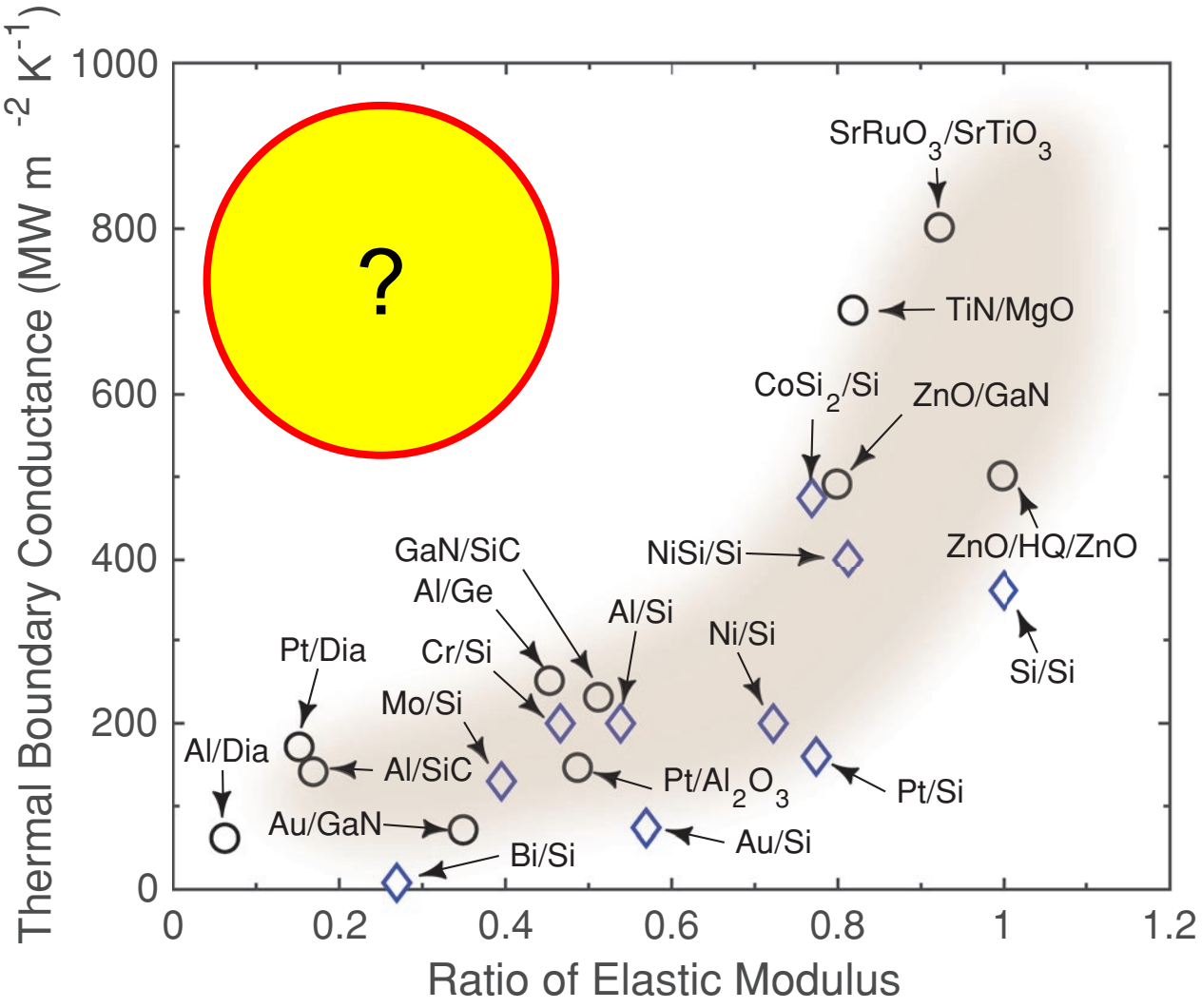
Gaskins *et al*. *Nano Letters* **18**, 7469 (2018)

- ZnO/GaN TBC highest TBC for crystalline/crystalline non-metal/non-metal to date
- Elastic models (semi-classical and atomistic) fail to capture high temp values
- Inelastic scattering? Interfacial modes? Robust landscape of directions can be explored with high quality, well controlled interfaces



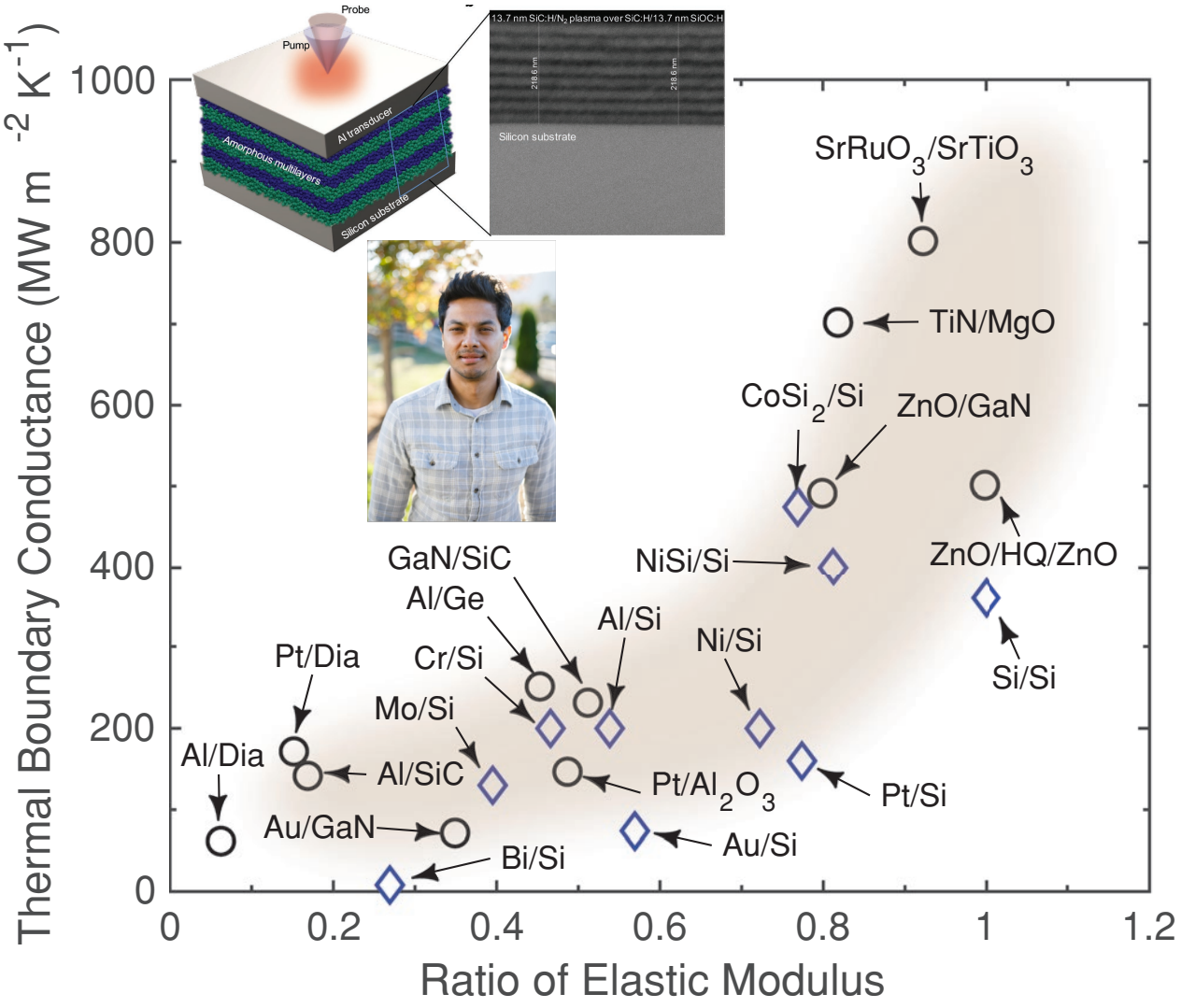
Looking ahead

Giri *et al*. *Advanced Materials* **30**, 1804097 (2018)



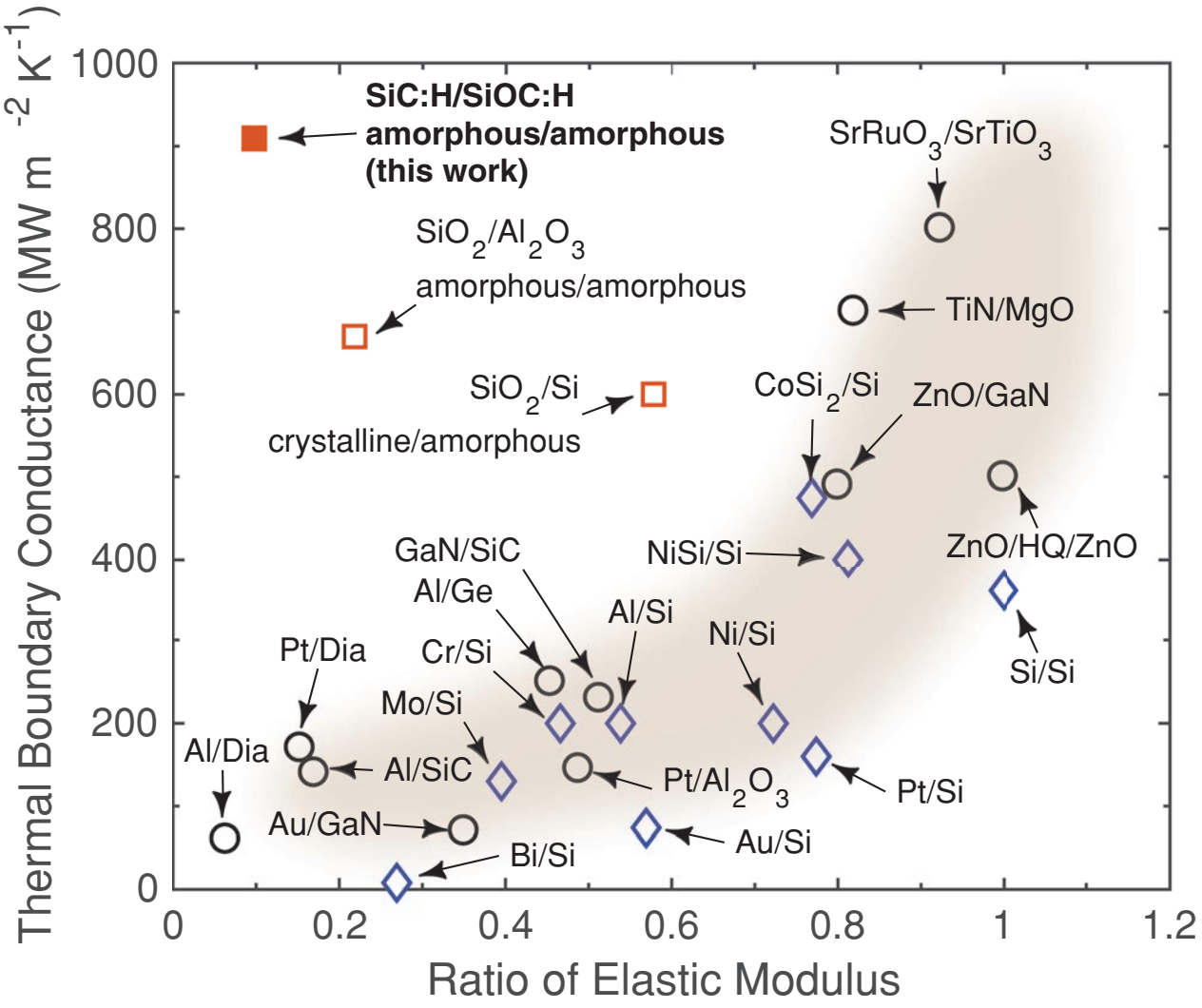
Looking ahead

Giri *et al*. *Advanced Materials* **30**, 1804097 (2018)

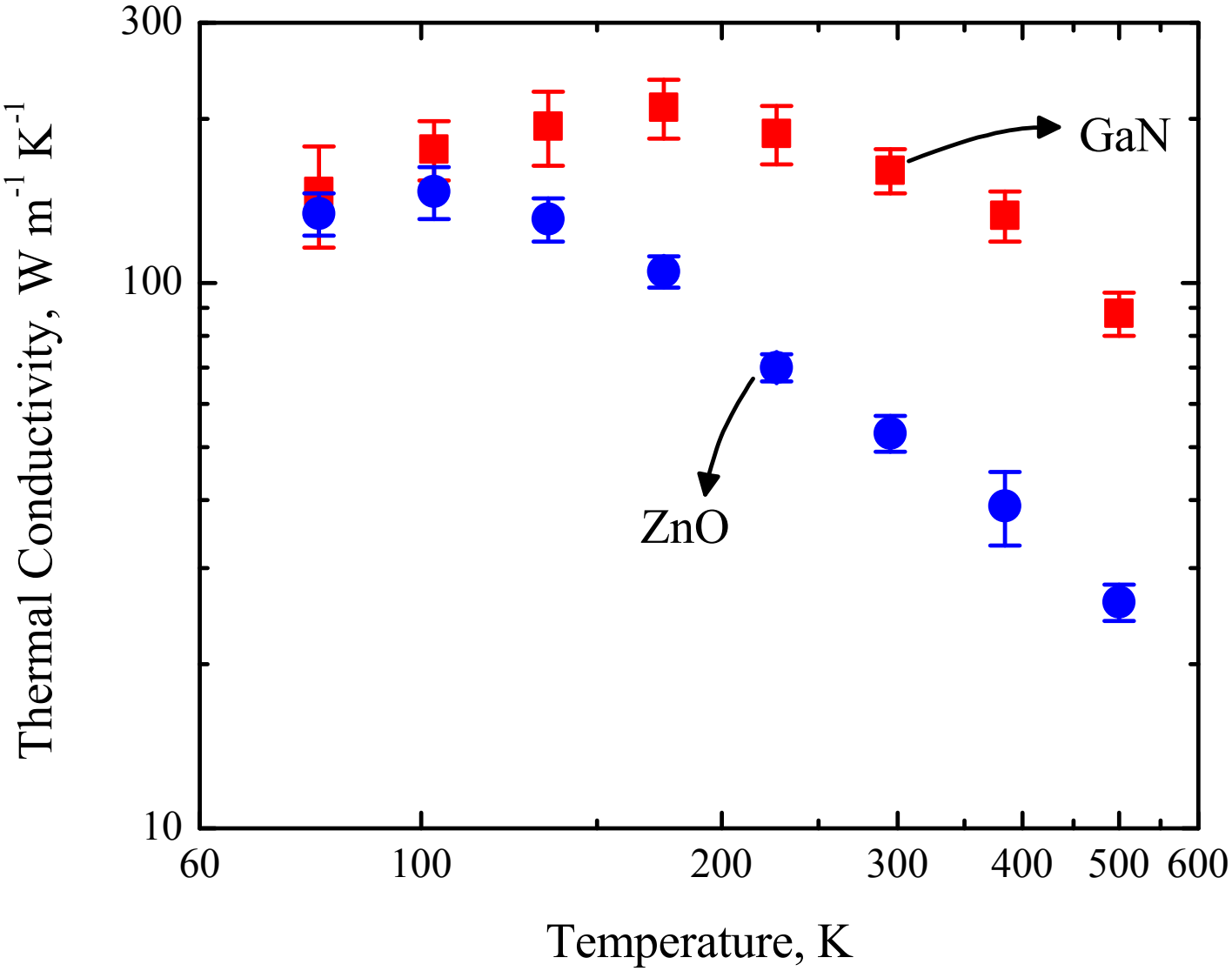


Looking ahead

Giri *et al*. *Advanced Materials* **30**, 1804097 (2018)

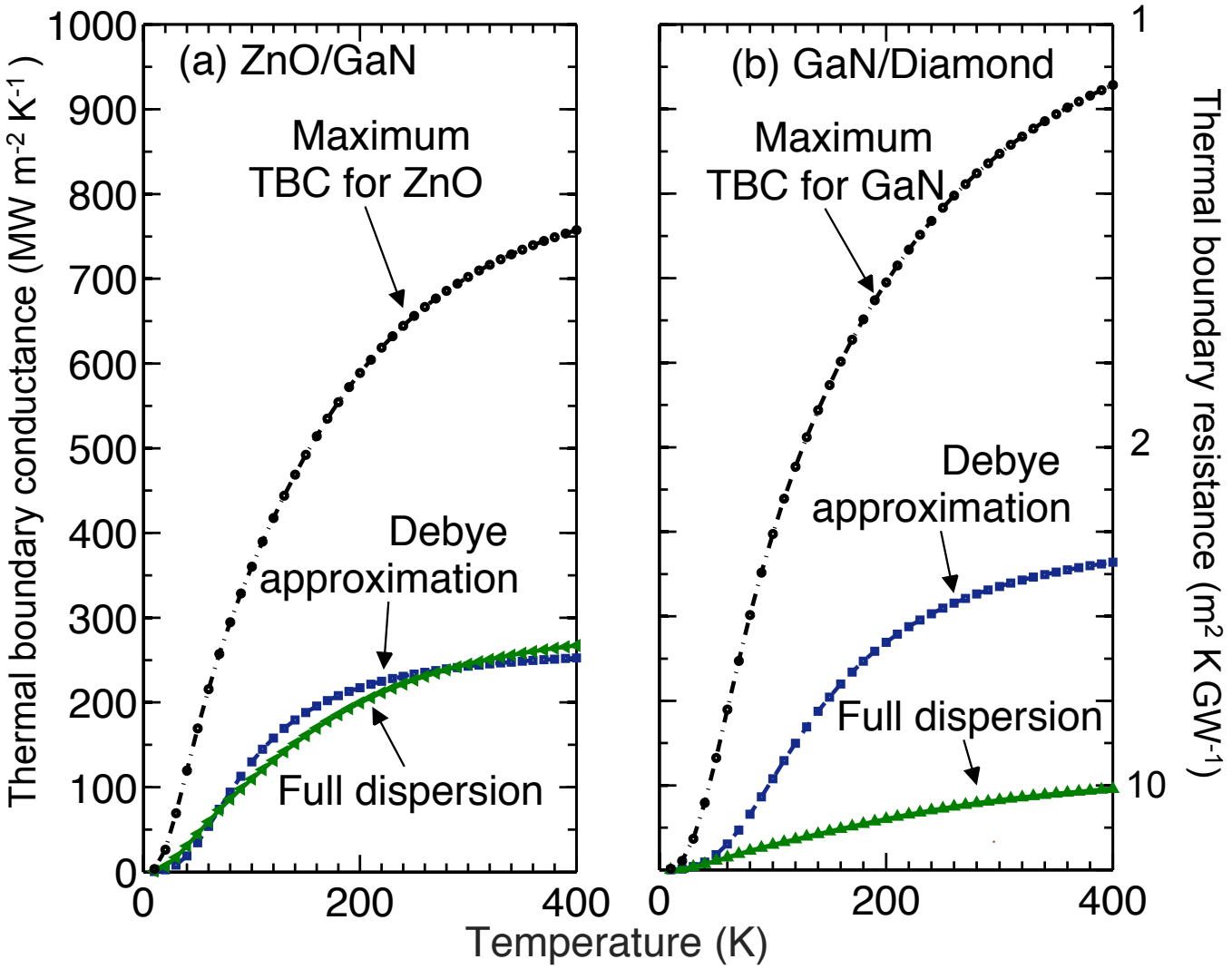


Thermal conductivity of GaN film on sapphire



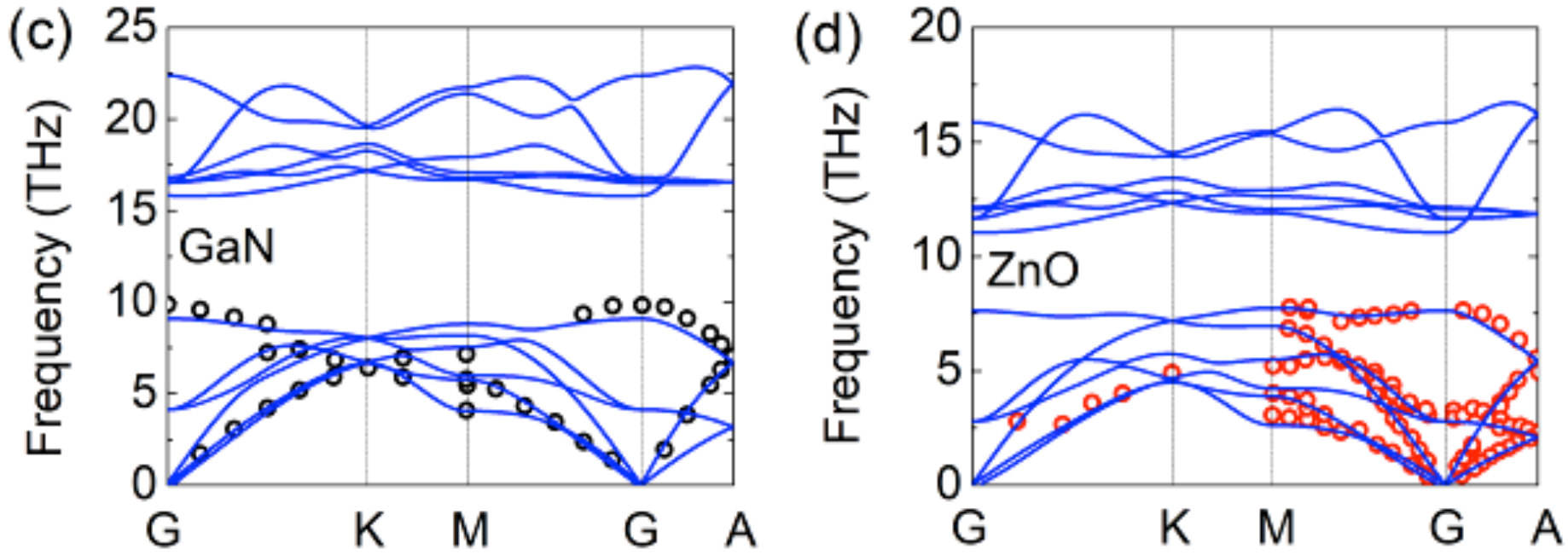
Gaskins *et al*. *Nano Letters* **18**, 7469 (2018)

In DMM calcs, should use full dispersion



Gaskins *et al*. *Nano Letters* **18**, 7469 (2018)

ZnO and GaN dispersion assumptions



Gaskins *et al*. *Nano Letters* **18**, 7469 (2018)