ARBEITSKREIS THERMOPHYSIK

in der GEFTA

# Multiscale modelling of phonon transport

Verena Fritz

Olga Natalia Bedoya-Martinez

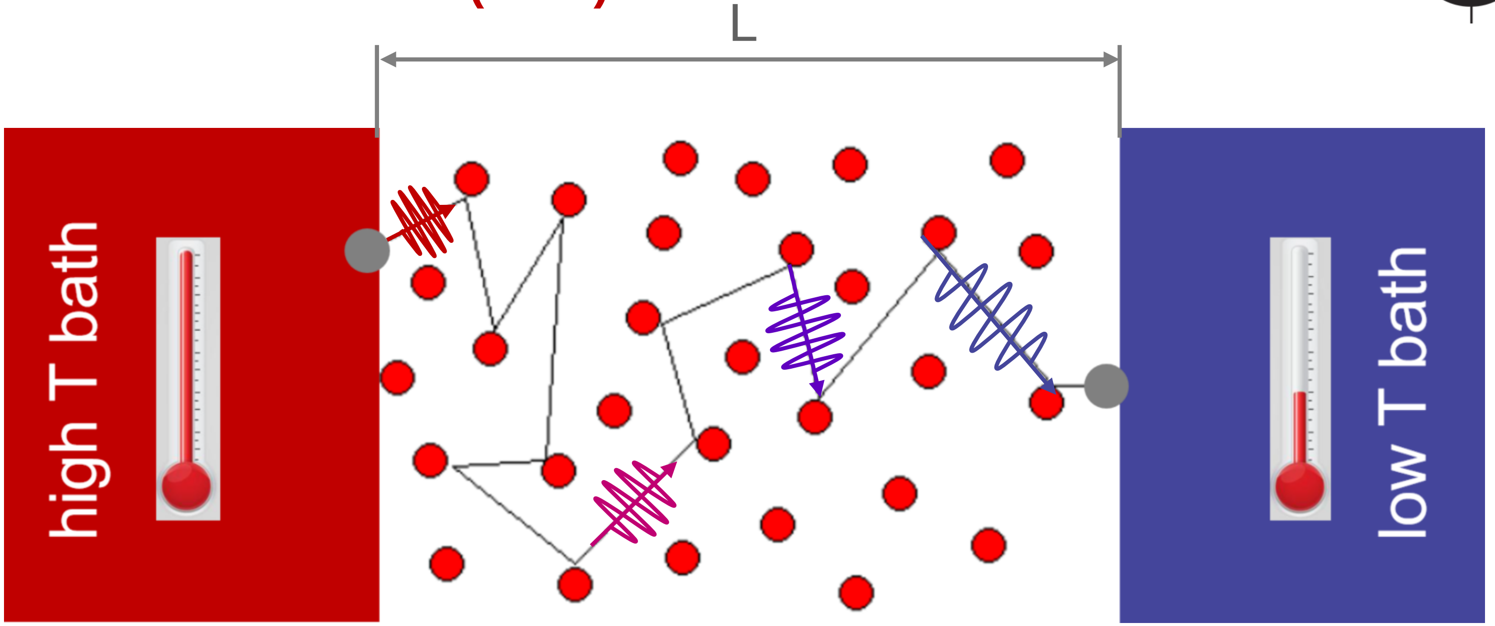
René Hammer*

www.mcl.at

rene.hammer@mcl.at

**Tagung des AK-Thermophysik, 08. – 09. April 2018, Leoben**

## The Phonon Gas Model (PGM)




$$C = \hbar\omega D \frac{\partial f}{\partial T} \qquad \vec{v} = \frac{\partial \omega}{\partial \vec{k}} \qquad \Lambda = \vec{v}\tau \qquad \mathbf{Kn} = \frac{\boldsymbol{\Lambda}}{\boldsymbol{L}}$$

THERMAL CONDUCTIVITY:

$$\kappa_\nu(\vec{k}) = C_\nu(\vec{k}) v_\nu(\vec{k}) \Lambda_\nu(\vec{k})$$

isotropic: $\omega(\vec{k}) = \omega(|\vec{k}|)$

$$\kappa_\nu(\omega) = C_\nu(\omega) v_\nu(\omega) \Lambda_\nu(\omega)$$

$$\kappa = \sum_\nu \int d\omega\, \kappa_\nu(\omega)$$

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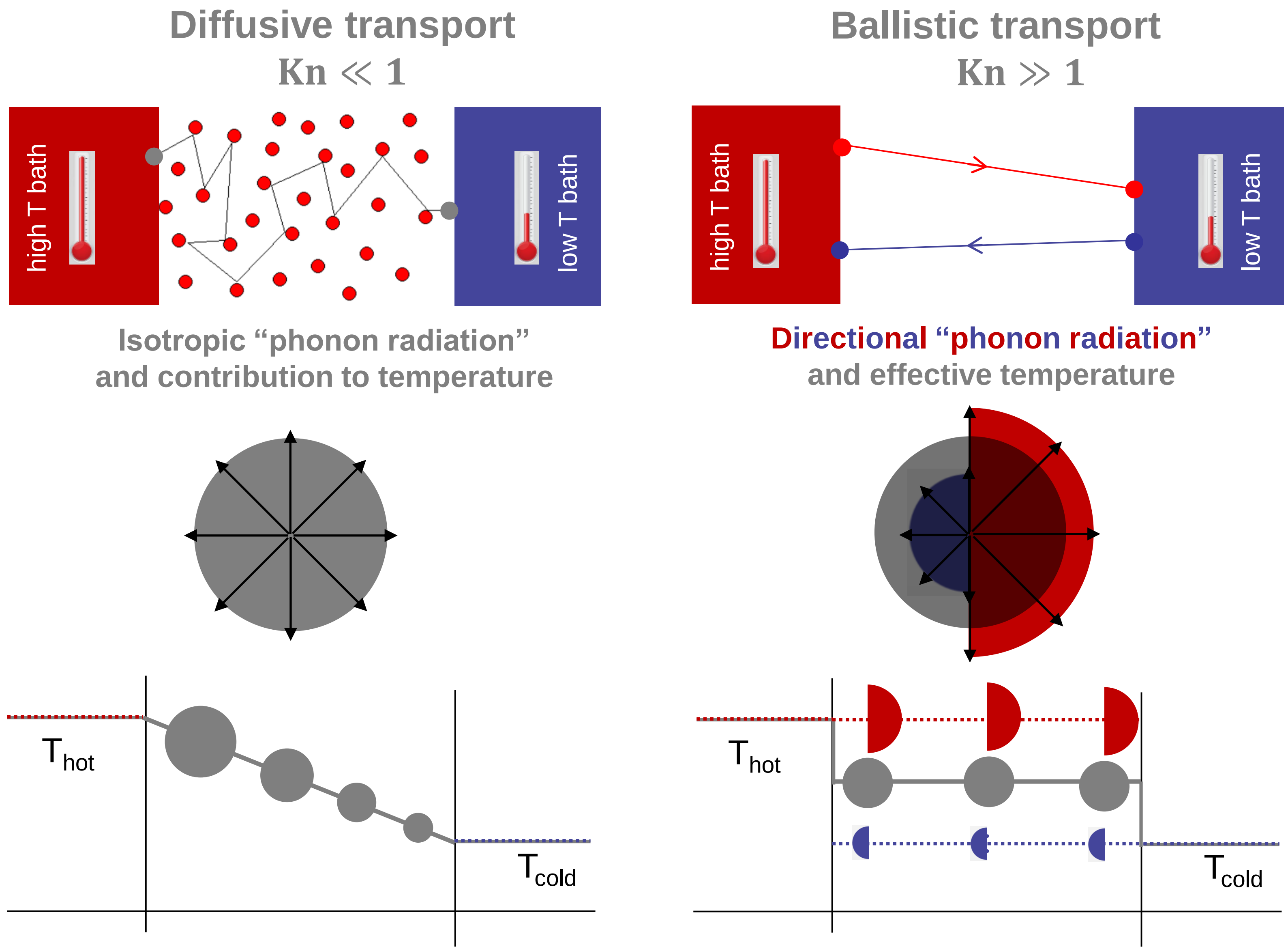
# Diffusive vs ballistic transport → Breakdown of Fourier's law

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# MOTIVATION: TDTR → MFP spectra (via pump spot size)

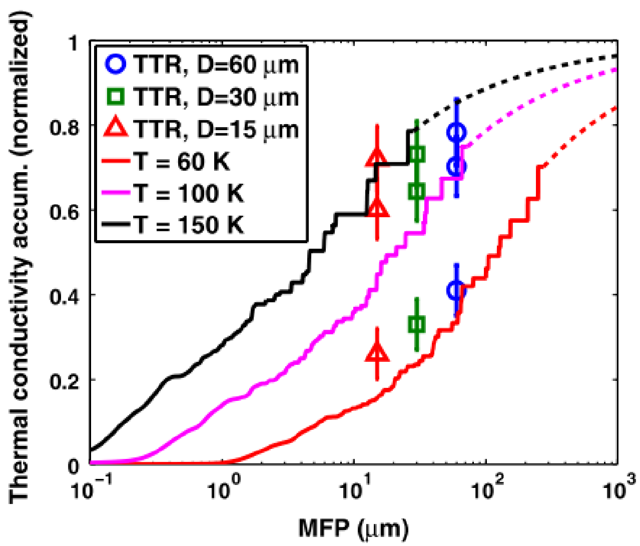
PRL 107, 095901 (2011) PHYSICAL REVIEW LETTERS week ending 26 AUGUST 2011

## Thermal Conductivity Spectroscopy Technique to Measure Phonon Mean Free Paths

A. J. Minnich,[1] J. A. Johnson,[2] A. J. Schmidt,[3] K. Esfarjani,[1] M. S. Dresselhaus,[4] K. A. Nelson,[2] and G. Chen[1,*]

..."Our approximation is that the ballistic group does not contribute to thermal transport due to the effectively infinite ballistic resistance; the thermal conductivity measured in the experiment is only due to the diffusive group..."

$$k_{\text{accum}}(\Lambda^*) = \int_0^{\Lambda^*} k_\Lambda d\Lambda = \int_0^{\Lambda^*} \frac{1}{3} C_\Lambda(\Lambda) v(\Lambda) \Lambda d\Lambda.$$




→ simplified assumption: phonons only contribute up to a certain cutoff MFP $\Lambda^*$:

# MOTIVATION: TDTR → MFP spectra

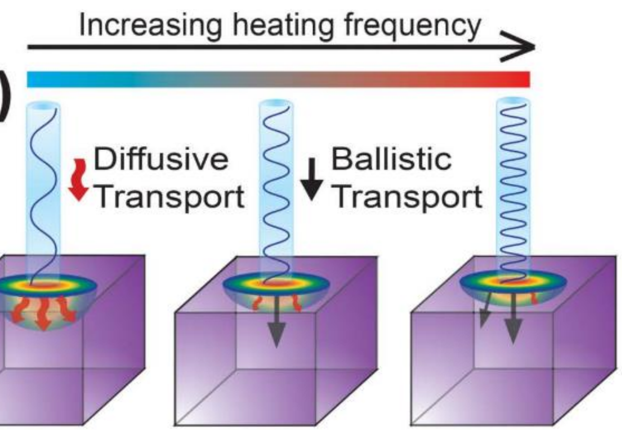
## (via modulation frequency)

SCIENTIFIC REPORTS | 3 : 2963 | DOI: 10.1038/srep02963

Universal phonon mean free path spectra in crystalline semiconductors at high temperature

Justin P. Freedman[1], Jacob H. Leach[2], Edward A. Preble[2], Zlatko Sitar[3], Robert F. Davis[1] & Jonathan A. Malen[1,4]

(d)

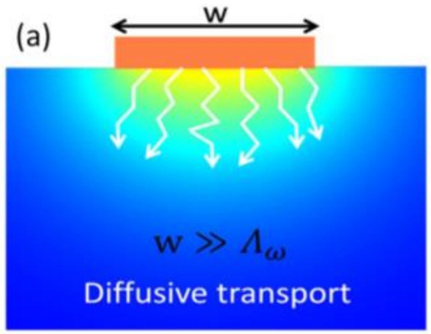


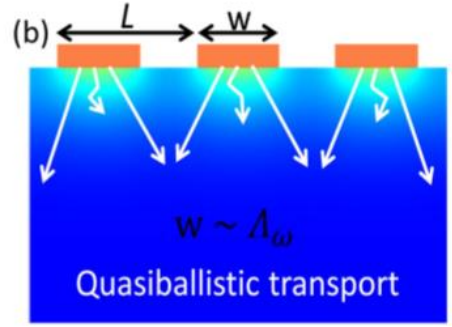

50% of thermal conductivity accumulation @ RT:

- GaN 1.0 ± 0.2 µm
- AlN 2.5 ± 0.8 µm
- SiC 4.2 ± 0.9 µm

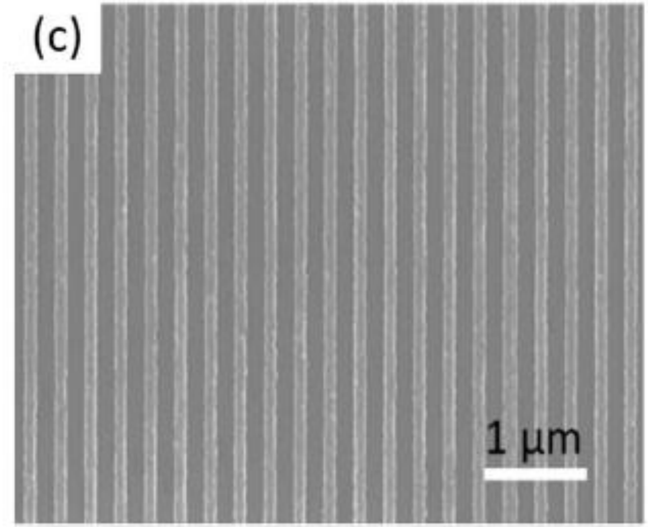
# MOTIVATION: TDTR → MFP spectra

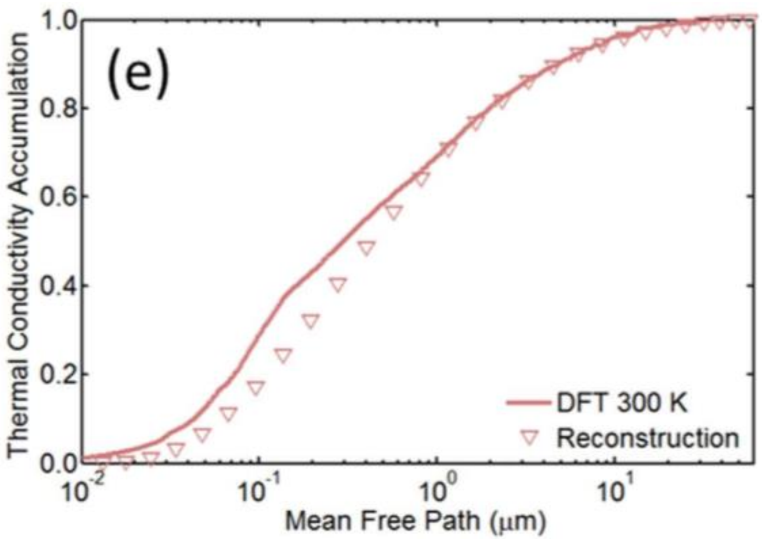
## (via heater structures)




Al grating on Si substrate



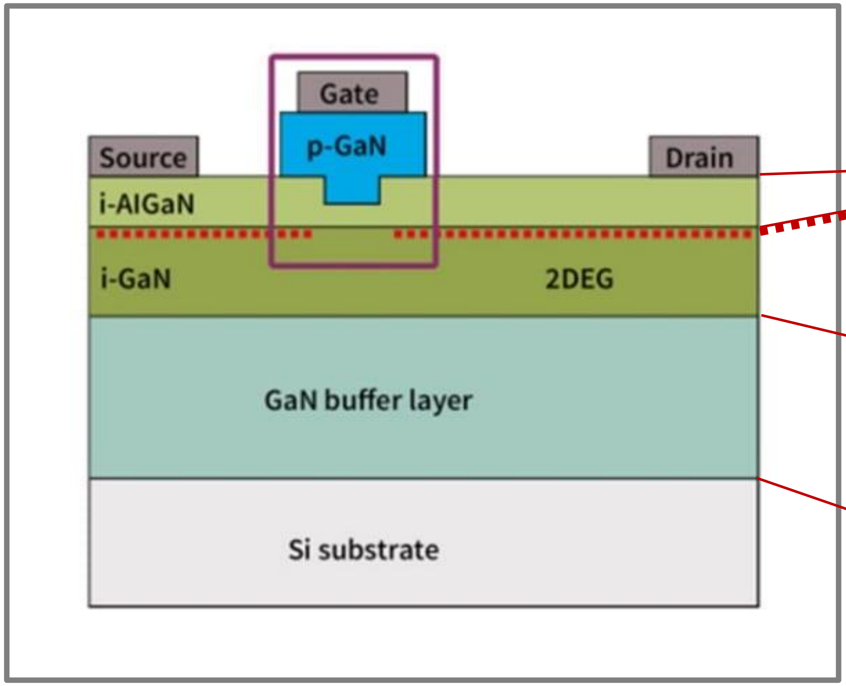

Zeng, Lingping, et al. "Measuring phonon mean free path distributions by probing quasiballistic phonon transport in grating nanostructures." *Scientific reports* 5 (2015): 17131.

$$k_{eff}(w) = \int_0^\infty S(\eta) f(\Lambda)\, d\Lambda \qquad \eta = \frac{\Lambda}{w}$$

Using suppression fuction $S(\eta)$ (derived from BTE) and lengthscale dependent thermal conductivity measured on for different metal linewidths $k_{eff}(w)$

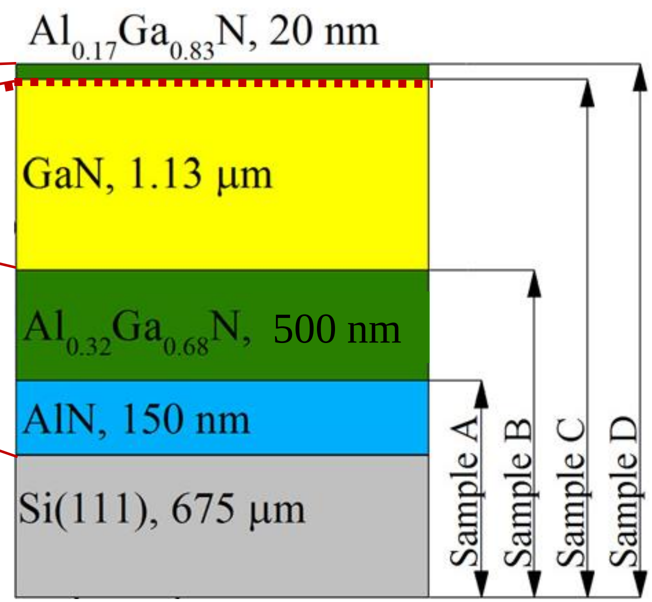
→ Cumulative phonon MFP distribution: $F(\Lambda) = \int_0^\Lambda f(\Lambda')\, d\Lambda'$

## E.g. Infineon “CoolGaN” device schematics:




*Reisinger et al., Appl. Phys. Lett. 111,162103 (2017)*

Example layer stack:

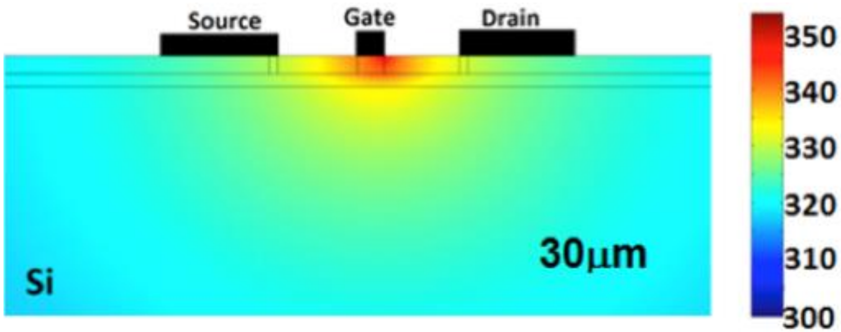



50% of thermal conductivity accumulation @ RT [DOI: 10.1038/srep02963]:

- GaN 1.0 ± 0.2 µm
- AlN 2.5 ± 0.8 µm

Compare Si 0.5 µm, from Henry and Chen, J. Comp. Theo. Nanosci 5, 1 (2008)

## E.g. Infineon “CoolGaN” device schematics:




Normally Fourier type simulations are used
(they are very wrong)

*J. Heat Transfer* 139(10), 102701

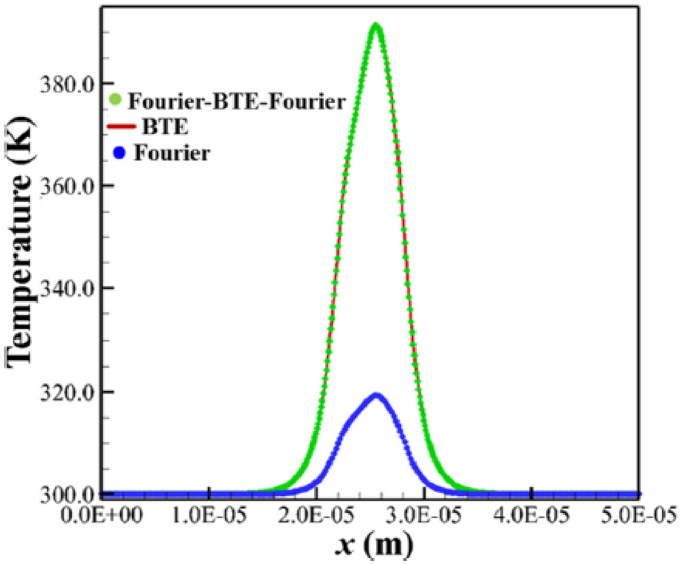



Fig. 4 Lattice temperature variation in the domain along the *x*-direction at the middle of the buffer (dotted line in the inset) at $y = 1.9 \times 10^{-6}\,\mu m$. The Fourier model significantly under-predicts the hot-spot temperature.

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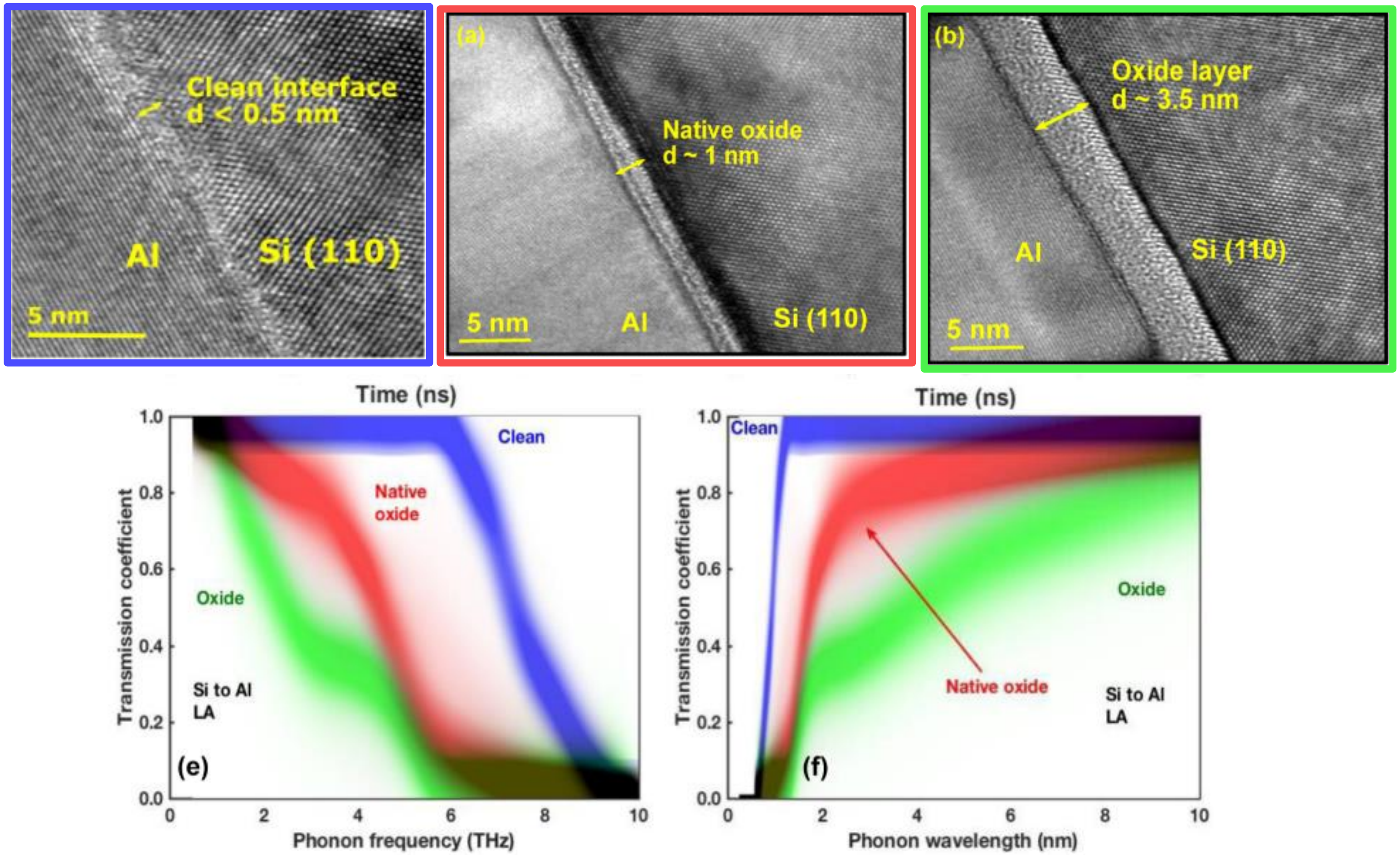
# MOTIVATION: TDTR → interface phonon transmission
## (enabled by ab initio computations)

PHYSICAL REVIEW B **95**, 205423 (2017)

**Experimental metrology to obtain thermal phonon transmission coefficients at solid interfaces**

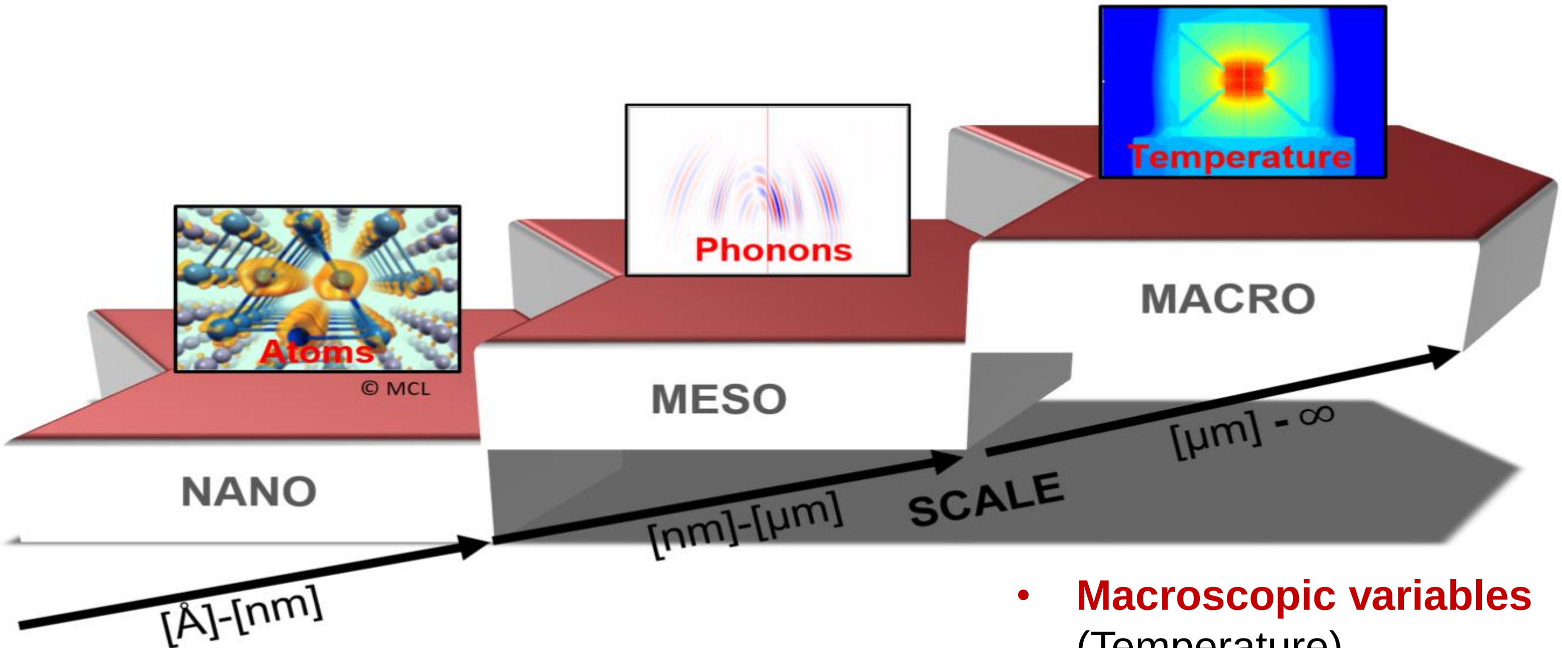
Chengyun Hua,[1] Xiangwen Chen,[2] Navaneetha K. Ravichandran,[3] and Austin J. Minnich[2,*]



# Multiscale modelling of phonon transport

## → Different scales → different descriptions

START FROM QUANTUM MECHANICS

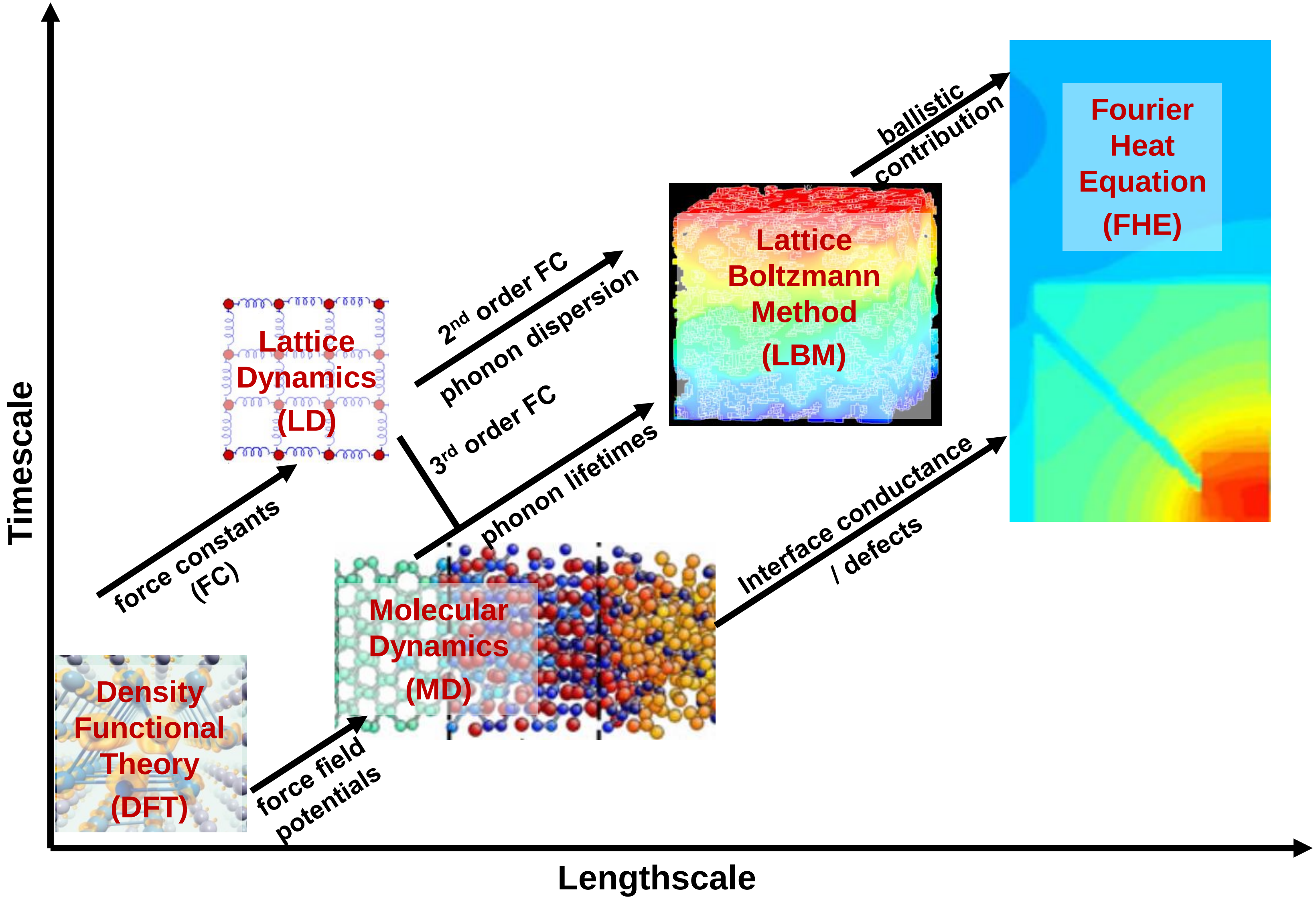



- **Position and momentum of all particles** (atoms)
- **Law of motion** (Newton)

- **Distribution function** (phonons)
- **Kinetic equation** (Boltzmann transport equation BTE)

- **Macroscopic variables** (Temperature)
- **Macroscopic transport equations** (Heat equation and beyond)

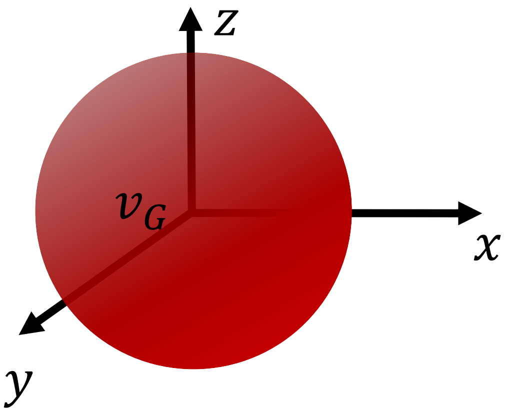
## Methods

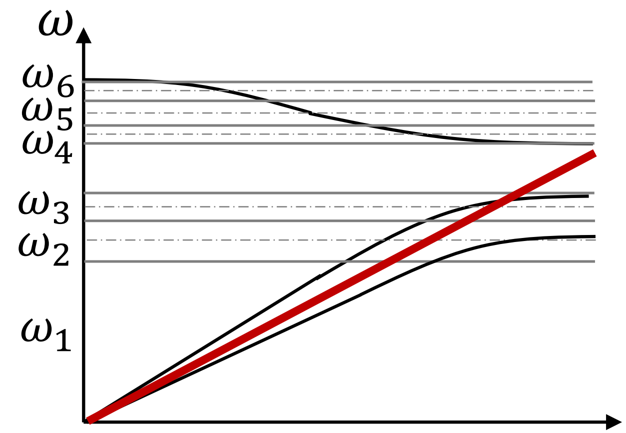

Timescale
Lengthscale
Density Functional Theory (DFT)
force constants (FC)
Lattice Dynamics (LD)
force field potentials
Molecular Dynamics (MD)
2nd order FC
phonon dispersion
3rd order FC
phonon lifetimes
Lattice Boltzmann Method (LBM)
ballistic contribution
Interface conductance / defects
Fourier Heat Equation (FHE)

# Lattice Boltzmann method (LBM)

- **Gray approximation**

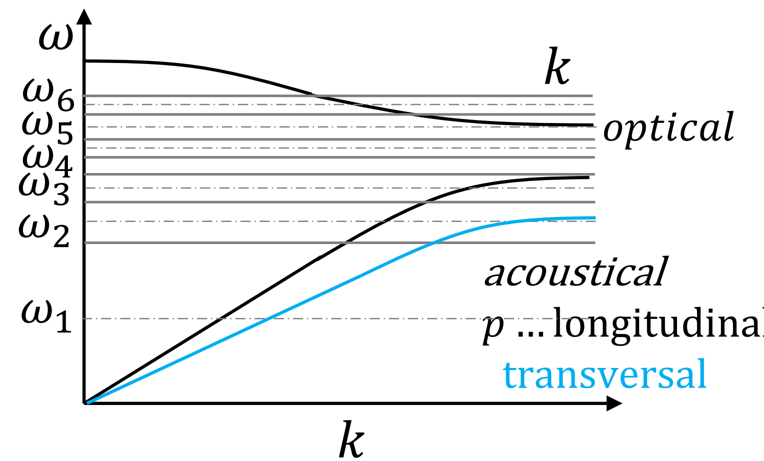
All modes are represented by one representative isotropic constant group velocity $v_G$




- **Beyond gray approximation → dispersion lattice Boltzmann**

Each direction, energy region and polarization has its own group velocity $v_i(\omega_j, p)$




Escobar, Rodrigo A., and Cristina H. Amon. "Thin film phonon heat conduction by the dispersion lattice Boltzmann method." *Journal of Heat Transfer* 130.9 (2008)

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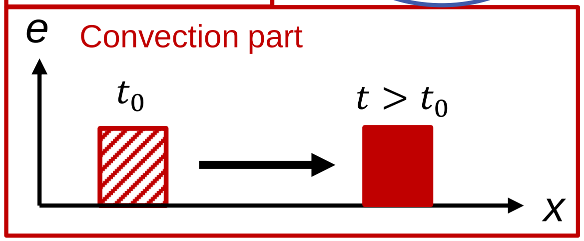
## Lattice Boltzmann method (LBM)

Boltzmann equation in energy formulation $e(T) = \sum_p \int f \hbar \omega_p D_p(\omega)\, d\omega$

$$\frac{\partial e}{\partial t} + \mathbf{v} \cdot \nabla e = -\frac{e - e^0}{\tau_r}$$

Scattering term
= driving force back to
equilibrium distribution




### Discretize direction (i) wise → Lattice Boltzmann

$$\frac{e_i(x, t + \Delta t) - e_i(x, t)}{\Delta t} + c_i \frac{e_i(x + \Delta x, t + \Delta t) - e_i(x, t + \Delta t)}{\Delta x} = -\frac{e_i(x, t) - e_i^0(x, t)}{\tau_r}$$

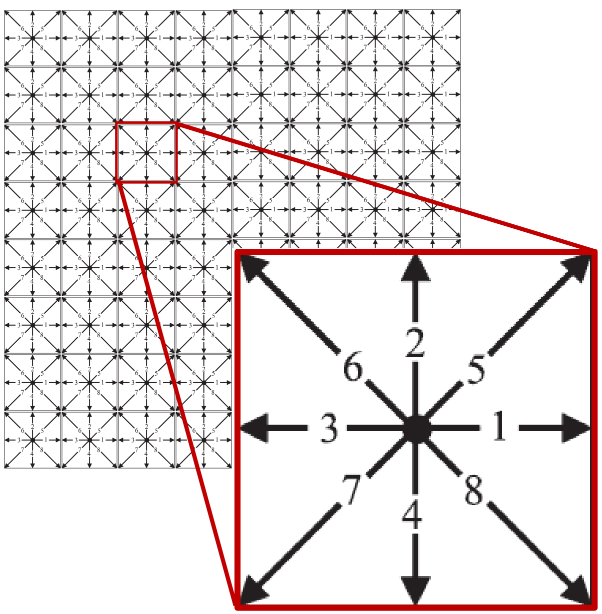
Convection ("streaming") Diffusion

$$e_1(x_i, y_j, t_{n+1}) = (1 - W) e_1(x_{i+1}, y_j, t_n) + W e^0(x_{i+1}, y_j, t_n)$$
$$e_2(x_i, y_j, t_{n+1}) = (1 - W) e_2(x_i, y_{j+1}, t_n) + W e^0(x_i, y_{j+1}, t_n)$$
$$e_3(x_i, y_j, t_{n+1}) = (1 - W) e_3(x_{i-1}, y_j, t_n) + W e^0(x_{i-1}, y_j, t_n)$$

.

.

$$e_8(x_i, y_j, t_{n+1}) = (1 - W) e_8(x_{i+1}, y_{j+1}, t_n) + W e^0(x_{i+1}, y_{j+1}, t_n)$$




$$e^0(x_i, y_j, t_n) = \sum_{Q=1}^{8} \frac{e_Q}{8}$$

Escobar, Rodrigo A. *et al.*, International Journal of Heat and Mass Transfer 49 (2006).



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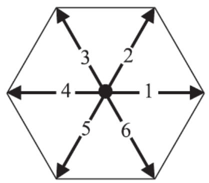
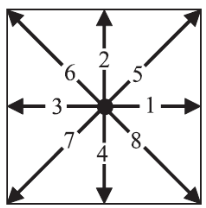
# LBM, (an)isotropy for high Knudsen numbers

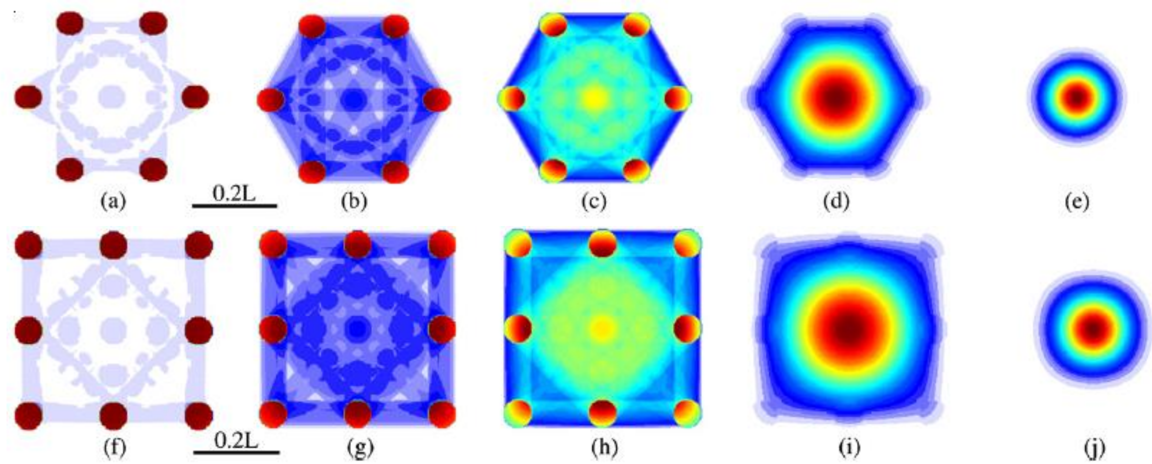
| LBM SCHEME | $Kn \approx 1.40$ | 0.42 | 0.14 | 0.05 | 0.014 |
|---|---|---|---|---|---|

*D2Q6*




*D2Q8*

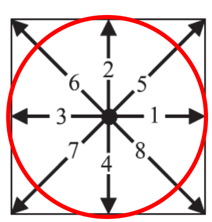


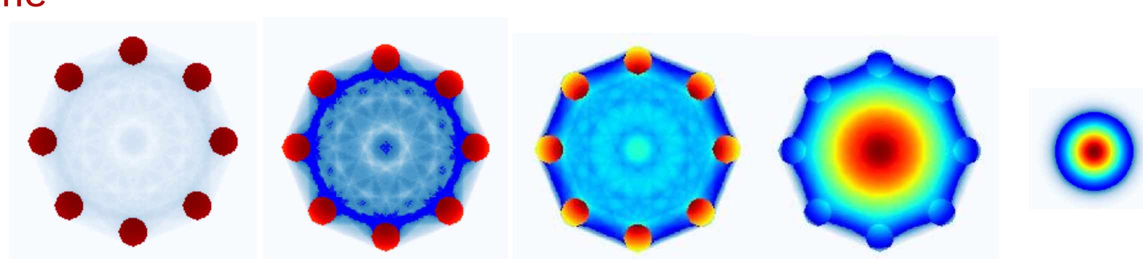




A. Nabovati et al. / Journal of Computational Physics 230 (2011) 5864–5876

our time adaptive scheme

*D2Q8i*



...in preparation

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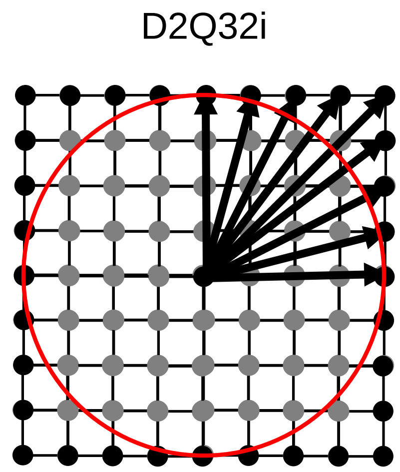
# Extending LBM to phonon transport towards the ballistic regime

- use lattice points further appart for more lattice directions





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# Extending LBM to phonon transport towards the ballistic regime

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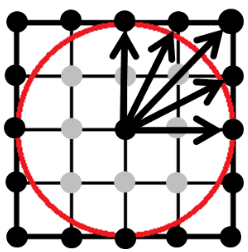
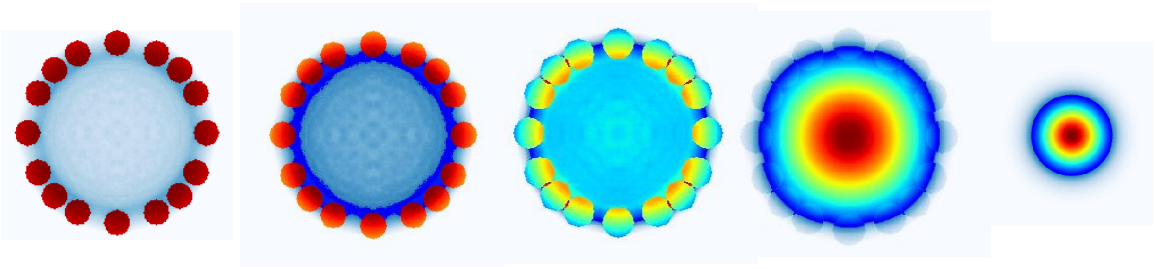
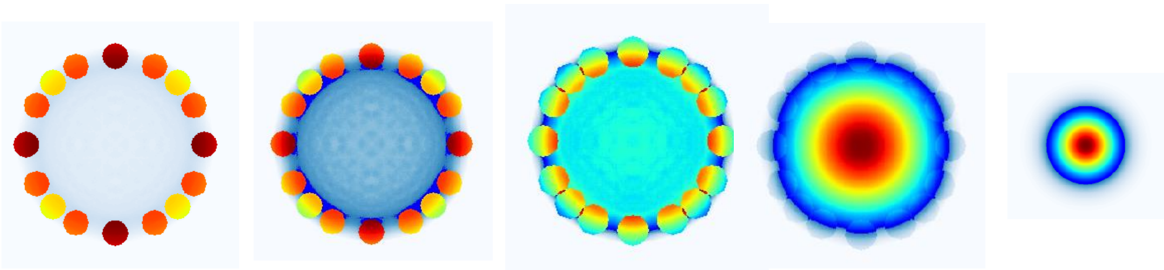
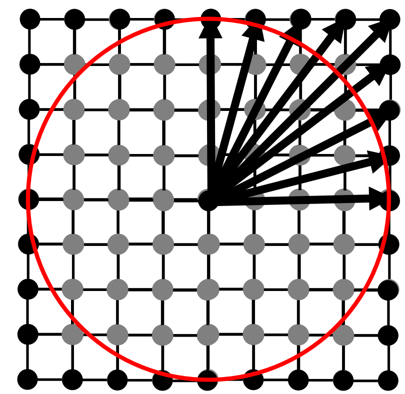
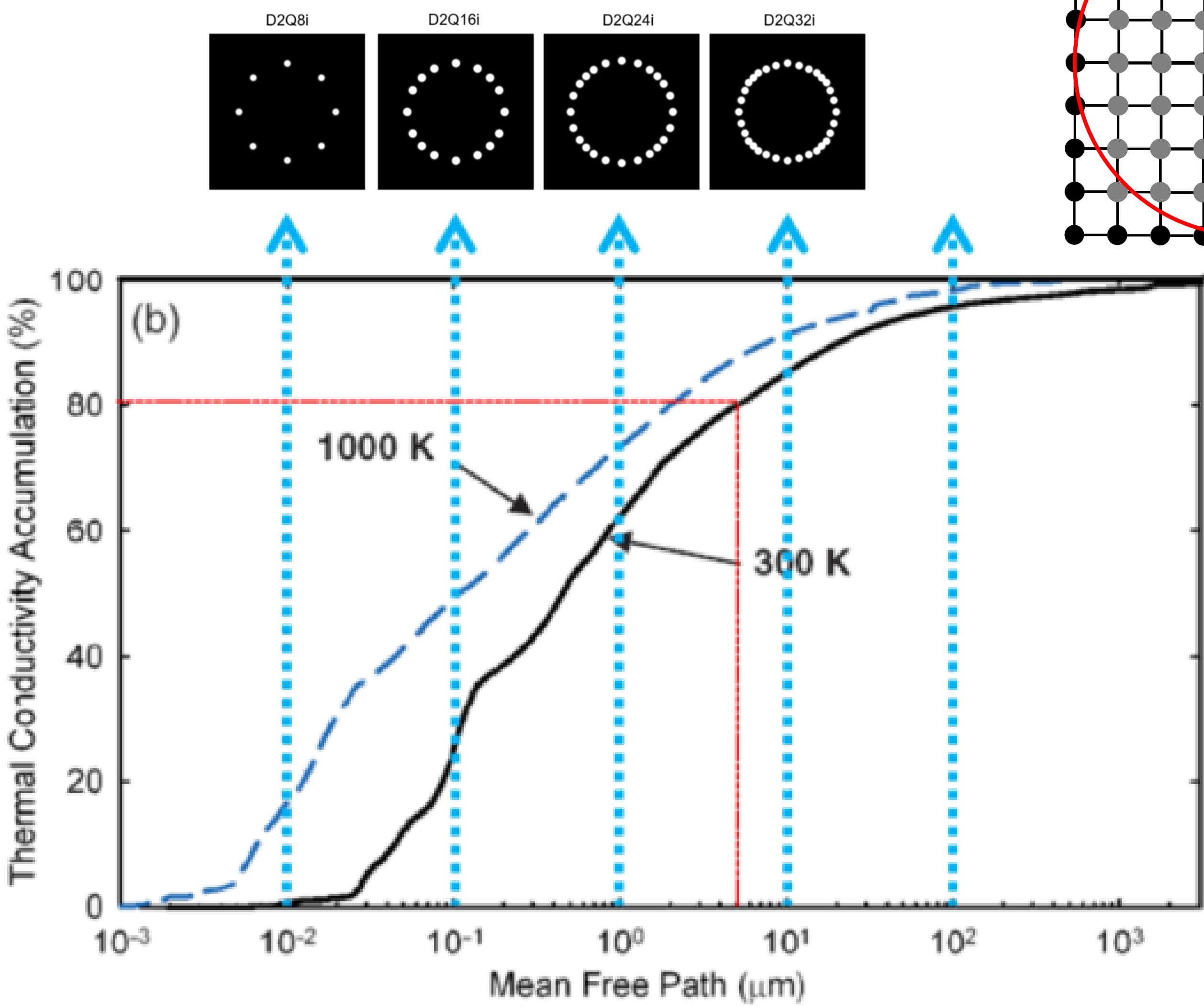
| LBM SCHEME | $Kn \approx 1.40$ | 0.42 | 0.14 | 0.05 | 0.014 |
|---|---|---|---|---|---|
| $D2Q16$  |  | | | | |
| $D2Q16$ *angular redistribution* |  | | | | |

## Extending LBM to phonon transport towards the ballistic regime

adoptive number of directional discretizations





## New paradigm: The Green Kubo Modal Analysis (GKMA)



Modal contribution to thermal conductivity

$$\kappa(n) = \frac{V}{k_B T^2} \int_0^\infty \langle \mathbf{Q}(n,t) \cdot \mathbf{Q}(0) \rangle \, \mathrm{d}t$$

Heat current in real space coordinates (from MD runs)

$$\mathbf{Q}(t) = \sum_n^{3N} \frac{1}{V} \sum_i \left[ E_i \dot{\mathbf{x}}_i(n,t) + \sum_j \left( -\nabla_{\mathbf{r}_i} \Phi_j \cdot \dot{\mathbf{x}}_i(n,t) \right) \mathbf{r}_{ij} \right]$$

Real space coordinates expressed in normal modes

$$\dot{\mathbf{x}}_j(t) = \sum_n \dot{\mathbf{x}}_j(n,t) = \frac{1}{m_j^{1/2}} \sum_n \mathbf{p}_j(n) \dot{X}(n,t)$$

(N atoms vibrating about their equilibrium sites → 3N normal modes)

GKMA = modal decomposition of heat current → mode-mode correlation ✔

PGM = requires well defined phonon properties ✘

W Lv and A Henry *New J. Phys.* 18 (2016) 013028

# THANK YOU
## MCL THERMAL TRANSPORT PIRATES

**Modelling** | **Experiments**

**DFT** | **MD** | **BTE** | **Fourier** | **TDTR** | **SThM**


Thomas Dengg


Verena Fritz


Katrin Fladischer


Verena Leitgeb


Jürgen Spitaler


Natalia Bedoya


René Hammer


Lisa Mitterhuber


Stefan Defregger

**Acknowledgement:**

The authors gratefully acknowledge the financial support under the scope of the COMET program within the K2 Center “Integrated Computational Material, Process and Product Engineering (IC-MPPE)” (Project No 859480). This program is supported by the Austrian Federal Ministries for Transport, Innovation and Technology (BMVIT) and for Digital and Economic Affairs (BMDW), represented by the Austrian research funding association (FFG), and the federal states of Styria, Upper Austria and Tyrol.

**Funded by:**

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