Fractional Calculus: A Possible Solution for Non-Fourier Heat Transfer Modeling?

Yanbao Ma

School of Engineering
University of California, Merced

Fractional Calculus Day @ UC Merced

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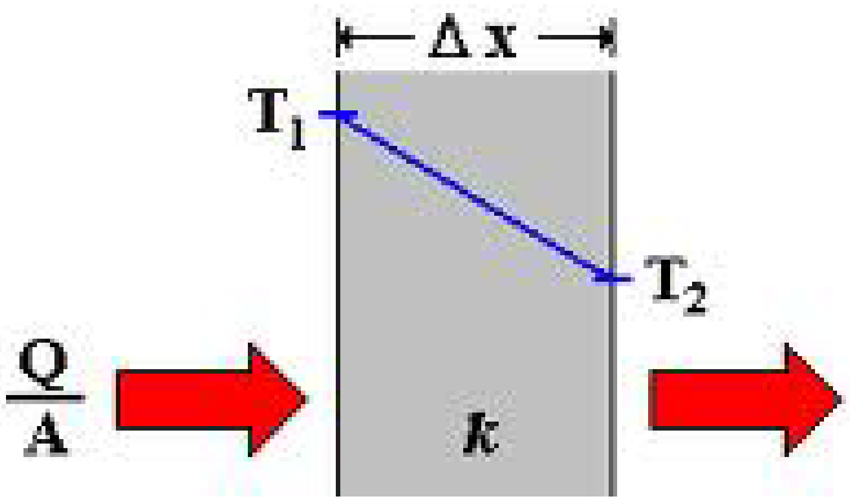
Outline

- Fourier's law for heat conduction
- Breakdown of Fourier's law in nanosystems
- Experimental evidence of ballistic heat transfer
- Modeling and numerical reconstruction of heat-pulse experiments
- Fractional calculus for non-Fourier heat transport?
- Summary

Fourier's Law

Joseph Fourier
1768-1830



$$Q = kA\left(\frac{T_1 - T_2}{\Delta x}\right)$$

$$\vec{q} = -k\nabla T$$

Fourier's Law: $\vec{q} = -k\nabla T$

- Fourier's law describes the **macroscopic** heat transport.
- There is **a lack of rigorous mathematical derivation** from first principles.

"Heat, like gravity, penetrates every substance of the universe, its rays occupy all parts of space … **The theory of heat** will hereafter form one of **the most important branches of general physics** … But whatever may be the range of <u>mechanical theories</u>, they **do not apply to the effects of heat.** These make up a special order of phenomena, which cannot be explained by the principles of motion and equilibria … "

------- Jean Baptiste Joseph Fourier

Fick's Law & Fourier's Law

Fourier's law: $\vec{q} = -k \nabla T$

"Heat Conduction Is a Can of Worms"

John Maddox, Nature, 1989, Vol. 338, pp 373

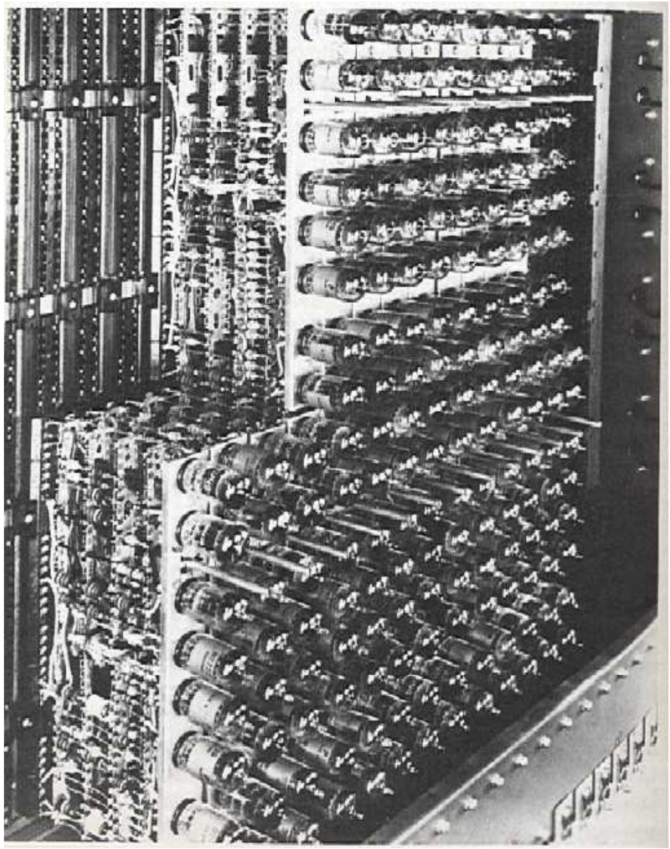
Fick's first law: $\vec{J} = -D \nabla \phi$

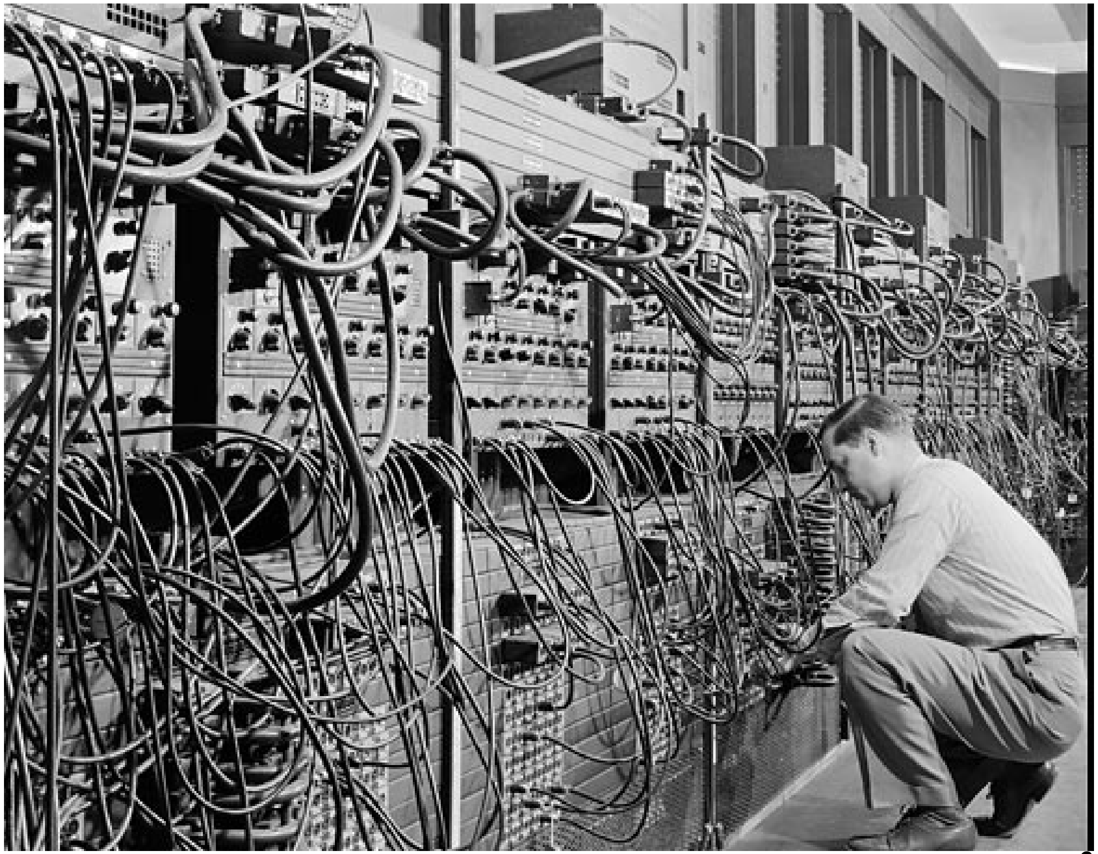
"A Bigger Can of Worms"

P. C. Malone, Nature, 1991, Vol. 349, pp 373

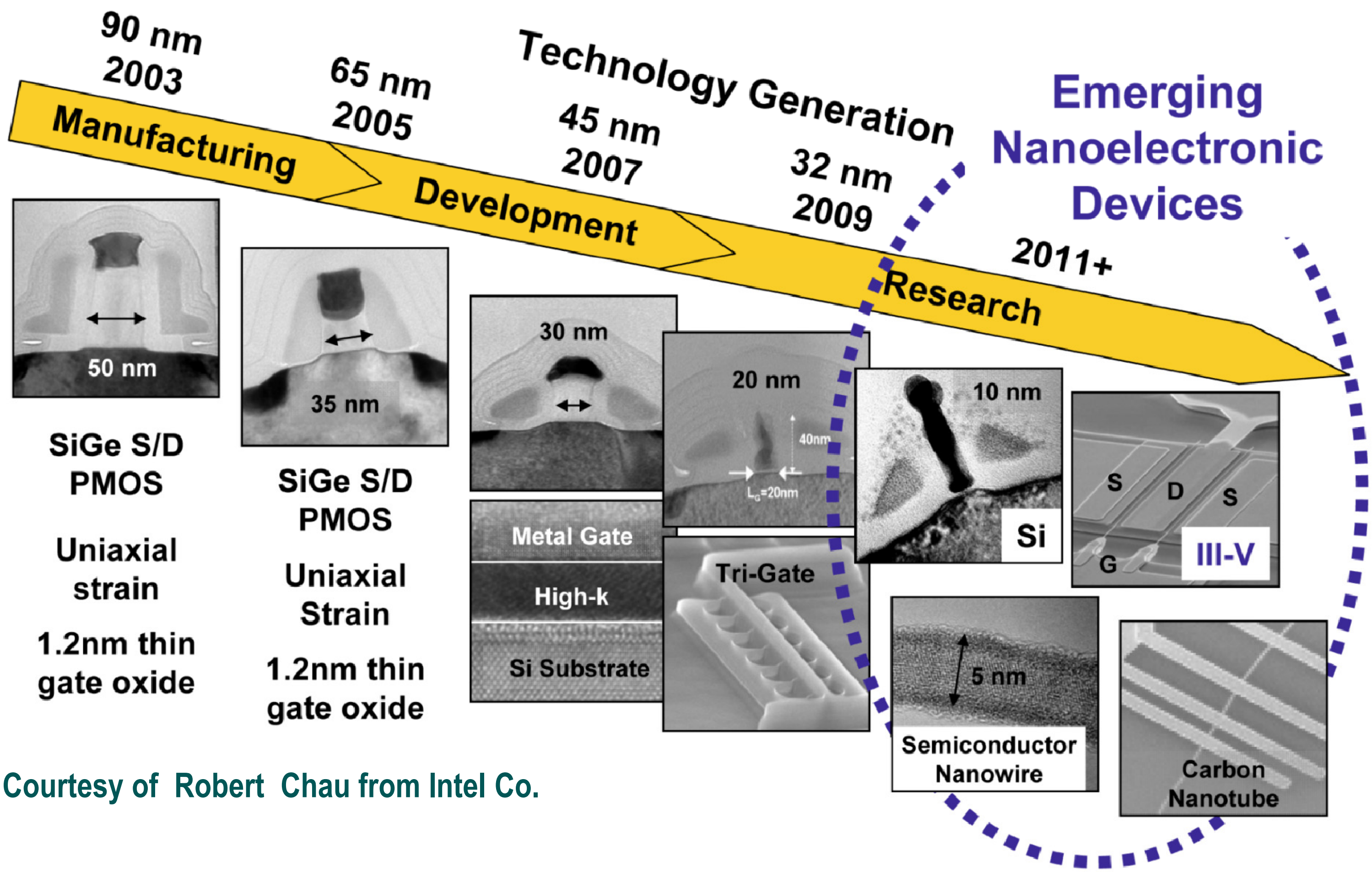
First Generation of Computer (1940-1959)

Vacuum tube



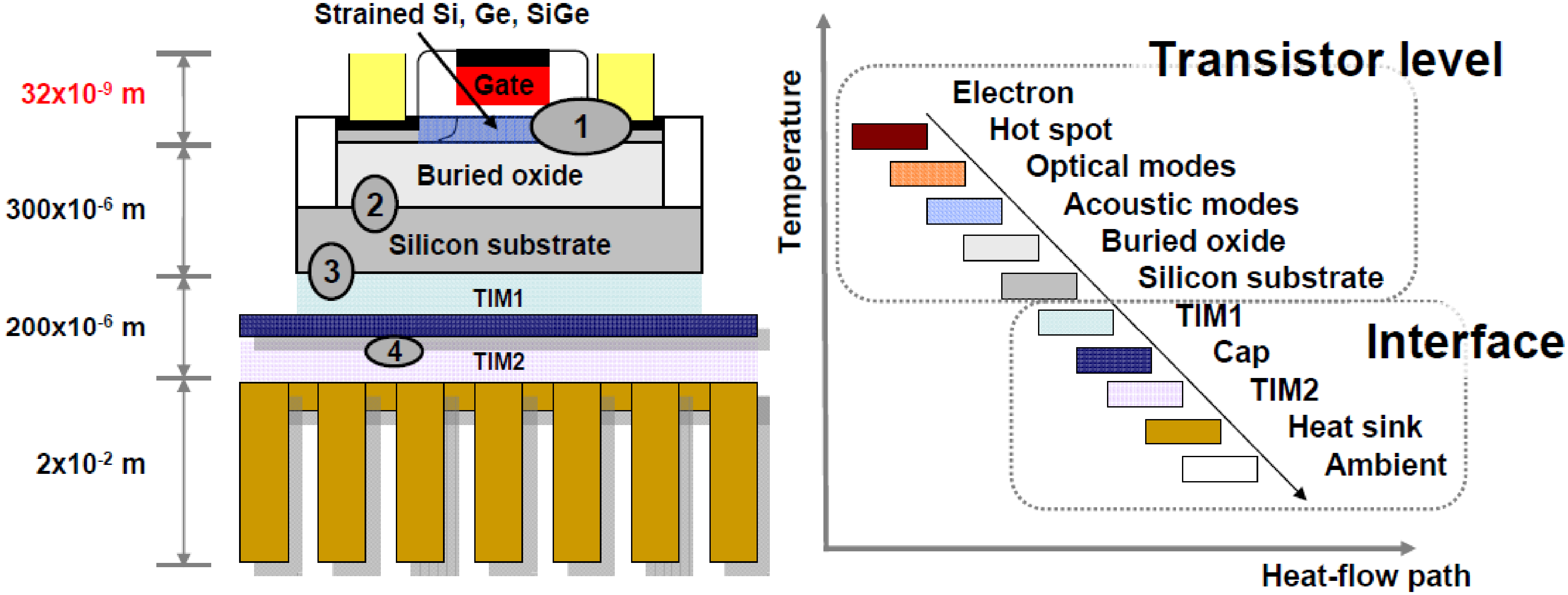


Micro/Nano Electronics



Courtesy of Robert Chau from Intel Co.

Thermal Management at Transistor Level



- **Each transistor is a heating source.**
- **Hot spot can be generated without efficient thermal management at transistor level.**

Amon CH, et al, Int. J. Heat & Mass Transfer, 2006, Vol. 49, 97-107.

Waste Thermal Energy

- **90%** of the world's power generated by heat engine using fossil fuel.

  Heat engine efficiency: **30%- 40%**

  15 Terawatts of heat is lost to the environment.

- Energy efficiency in transportation: **20%**

  & **700 Gigawatts** rejected as waste heat.

Thermoelectric Energy Conversion

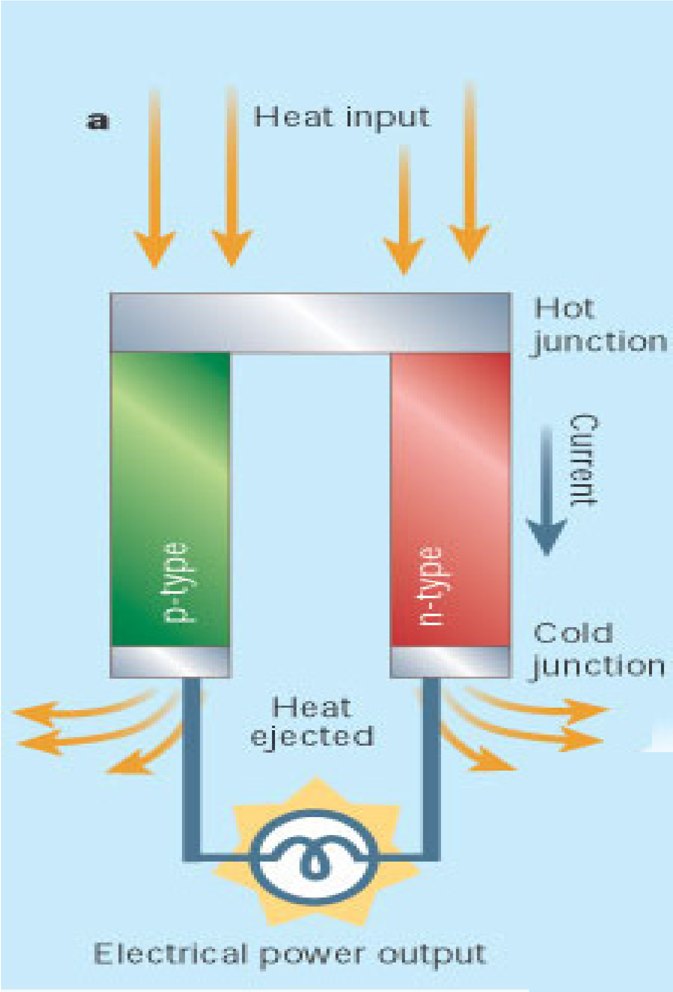


Figure of Merit Z:

$$Z = \frac{\sigma S^2}{\kappa}$$

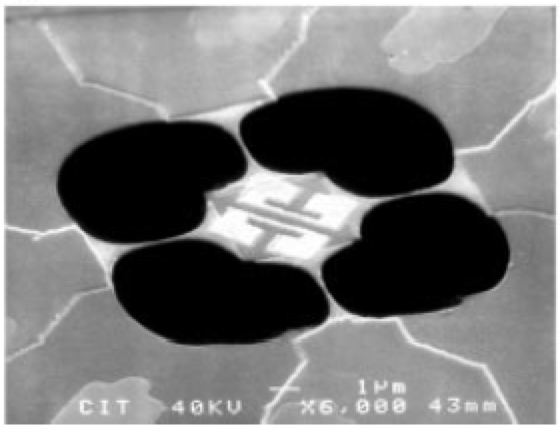
σ: electrical conductivity

κ: thermal conductivity

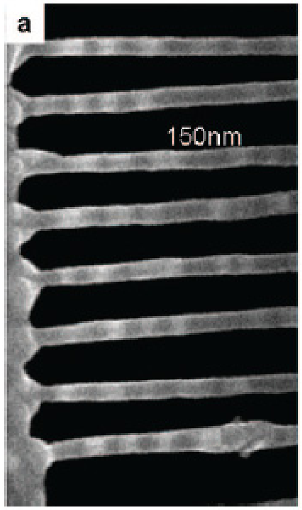
S: Seebeck coefficient

***Cronin Vining, Nature* 2001, 413, 577-578**

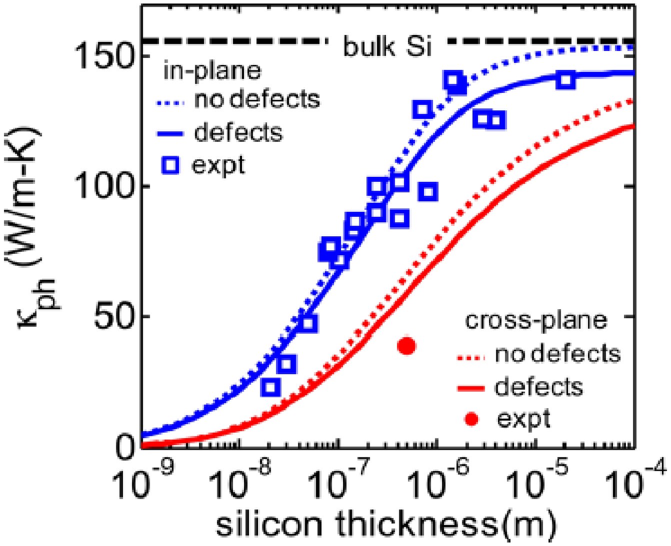
Thermoelectric Nano-Materials



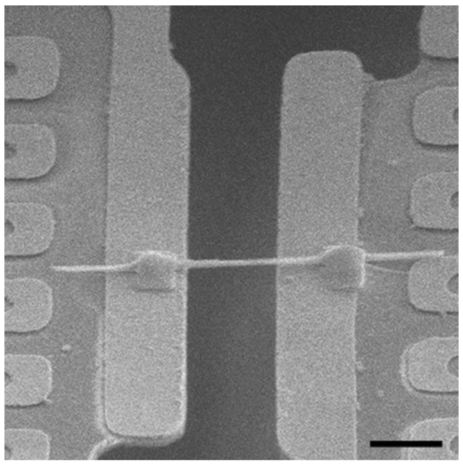
Schwab, Nature, 2000, v404, 974-977

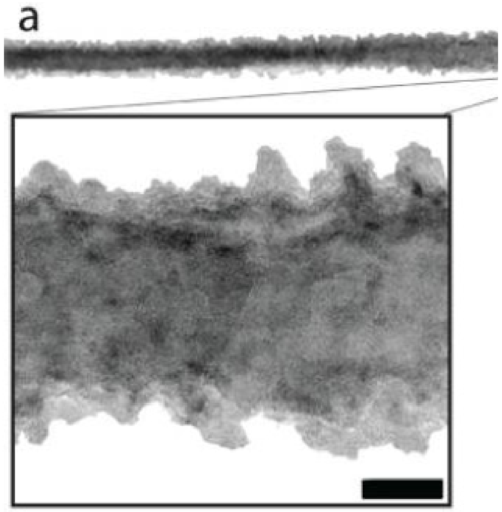


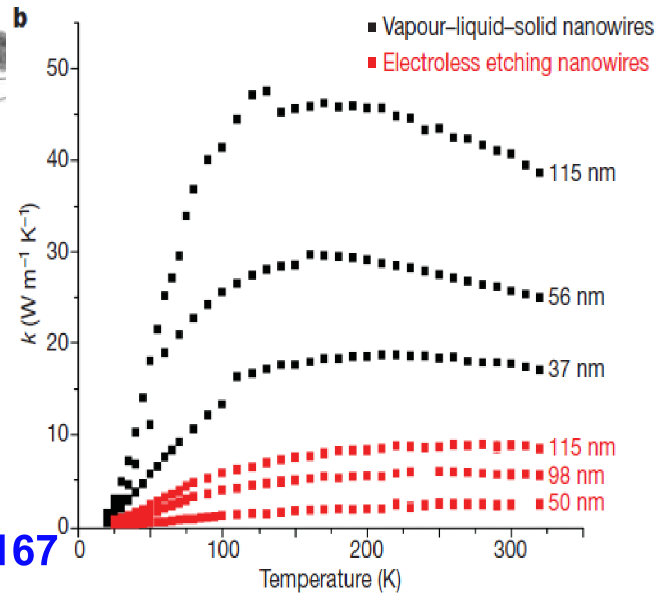
Huang et al, ACS Nano, 2009, v3, 721



Jeong et al, J. Appl. Phy, 2012, v111, 093708







Hochbaum et al, *Nature* 2008, Vol. 451, 163-167

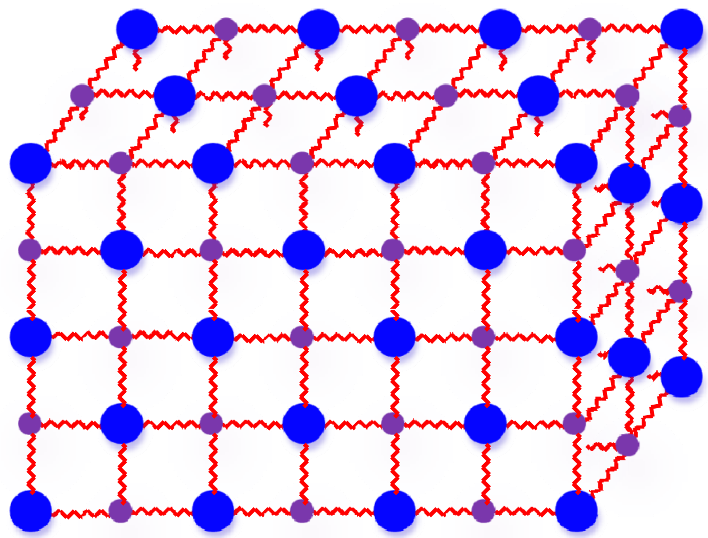
Breakdown of Fourier's Law

Geometry-/Size- dependent thermal conductivity →

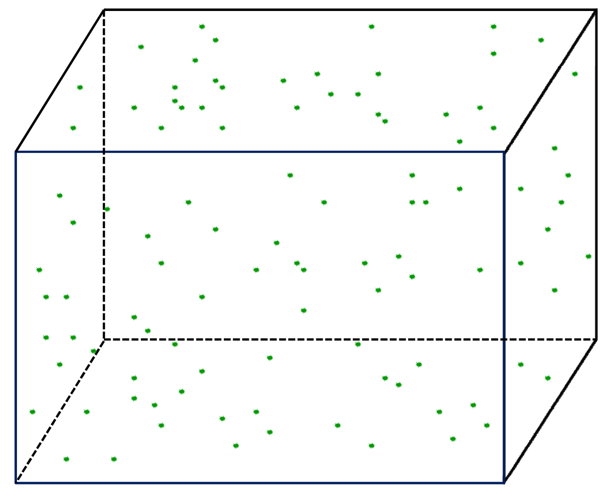
Breakdown of Fourier's law

What's the new law for non-Fourier heat transport?

Microscopic Heat Transfer



Lattice vibration



Phonon gas model

(Phonon: Quantization of Vibration Energy)

- **Diffusive Heat Transport:**

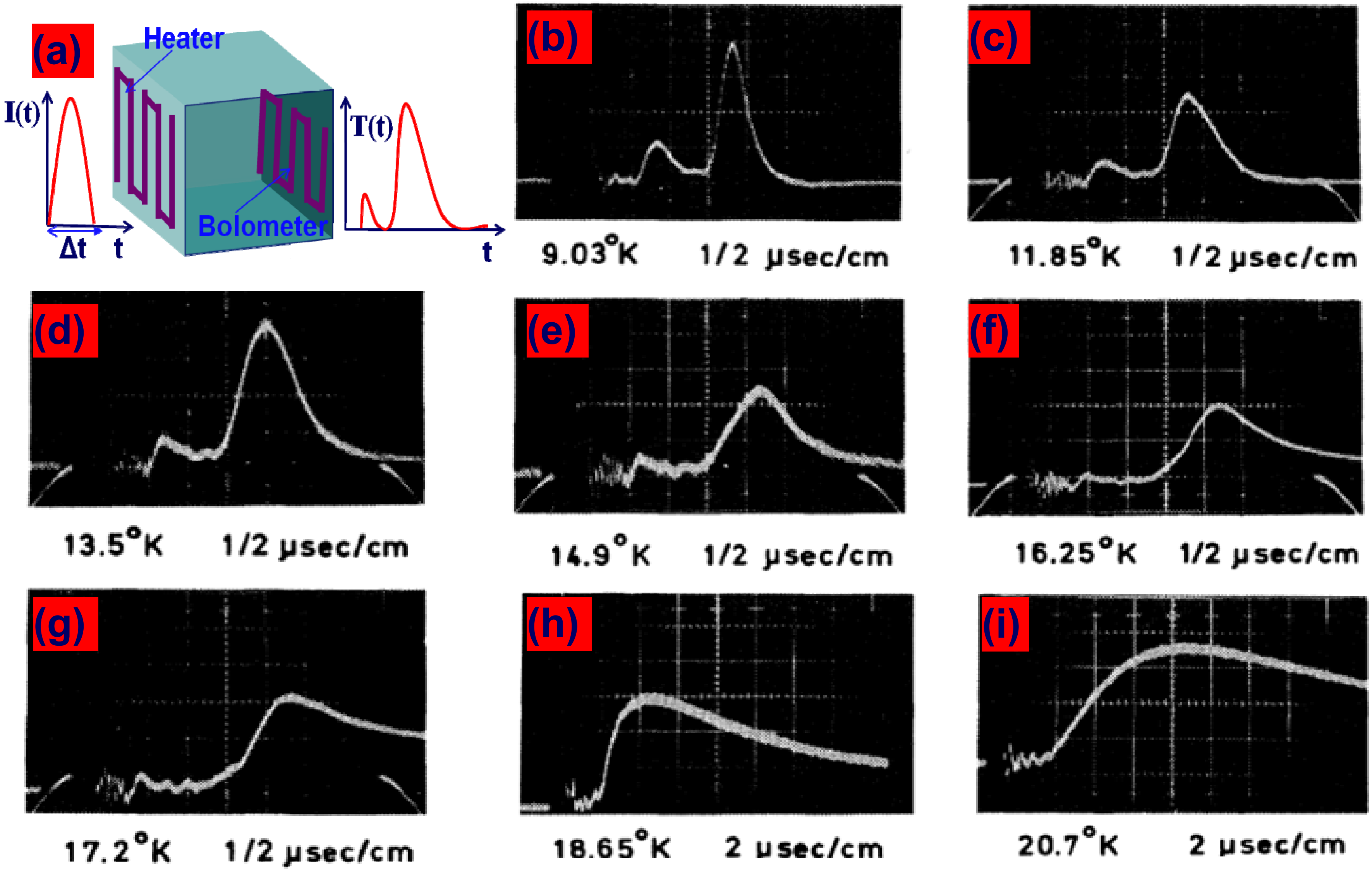
  System size >> Phonon Mean Free Path

- **Ballistic Transport (significant in nanosystems):**

  System size ≤ Phonon Mean Free Path (MFP)

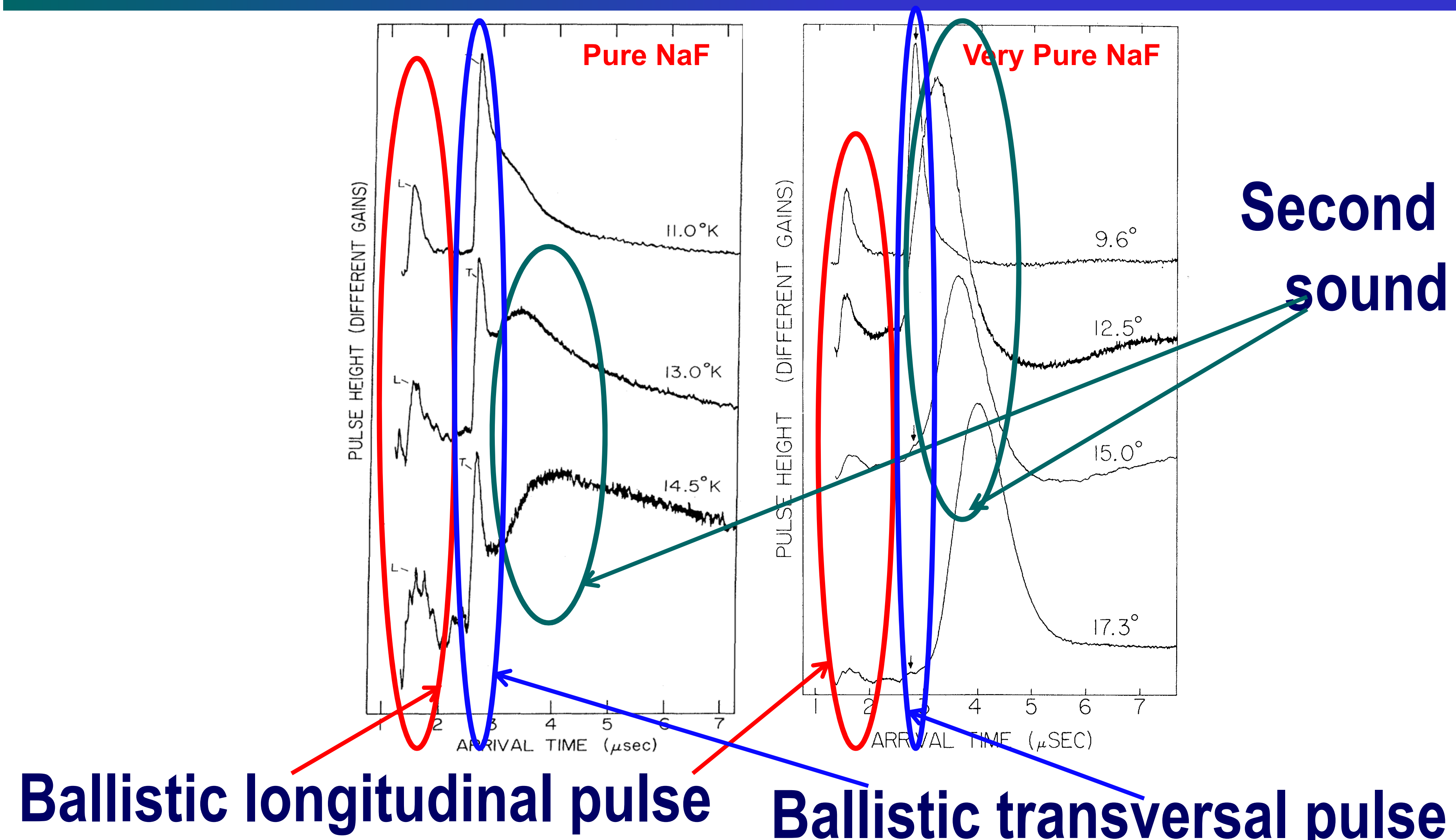
Direct Evidence of Ballistic Heat Transfer

Heat-Pulse Experiments at Low Temperatures



McNelly, PhD. Thesis, 1974

Identification of Thermal Waves



Jackson & Walker, Phys. Rev. B, Vo. 3, 1971;Jackson et al., Phy. Rev. Lett., v 25, 1970

Numerical Reconstruction of Heat-Pulse Experiments

Rogers' Viscous Phonon Gas Model

- **Navier-Stokes Equation for Fluid Dynamics**

$$\rho \frac{\partial \vec{u}}{\partial t} + \rho \vec{u} \cdot \nabla \vec{u} = -\nabla p + \mu \nabla^2 \vec{u} + (\zeta + \frac{1}{3}\mu)\nabla(\nabla \cdot \vec{u})$$

- **Evolution Equation for Heat Flux:**

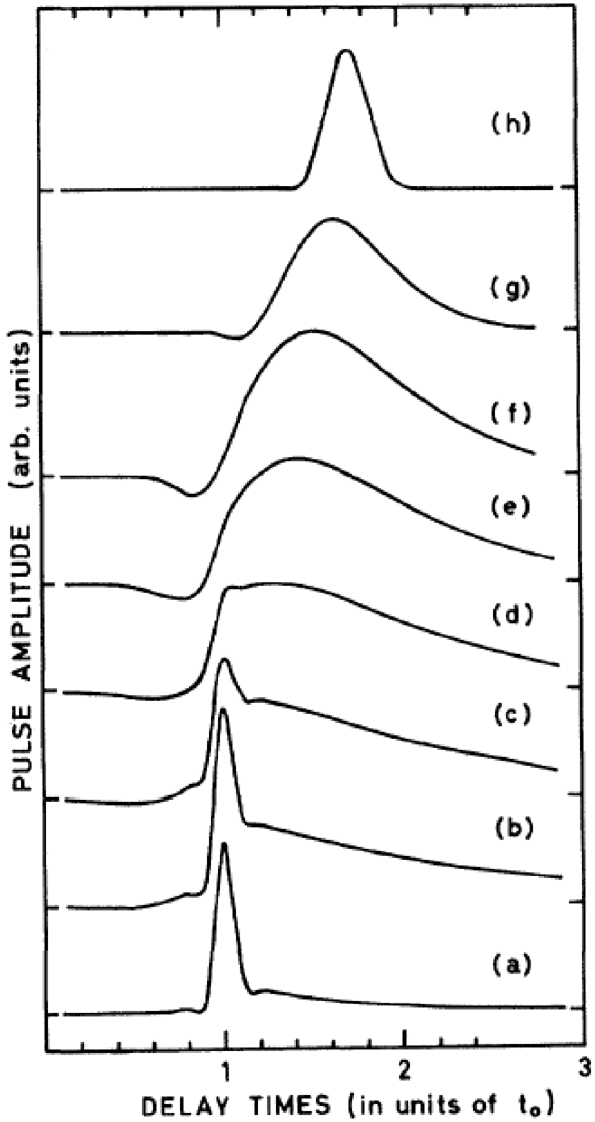
$$\frac{\partial \vec{q}}{c_1^2 \partial t} = \frac{1}{3}\nabla E - \frac{\vec{q}}{c_1^2 \tau_R} + \left[\mu_g \nabla^2 + (\zeta_g + \frac{1}{3}\mu_g)\nabla(\nabla \cdot)\right]\left(\frac{\vec{q}}{e}\right)$$

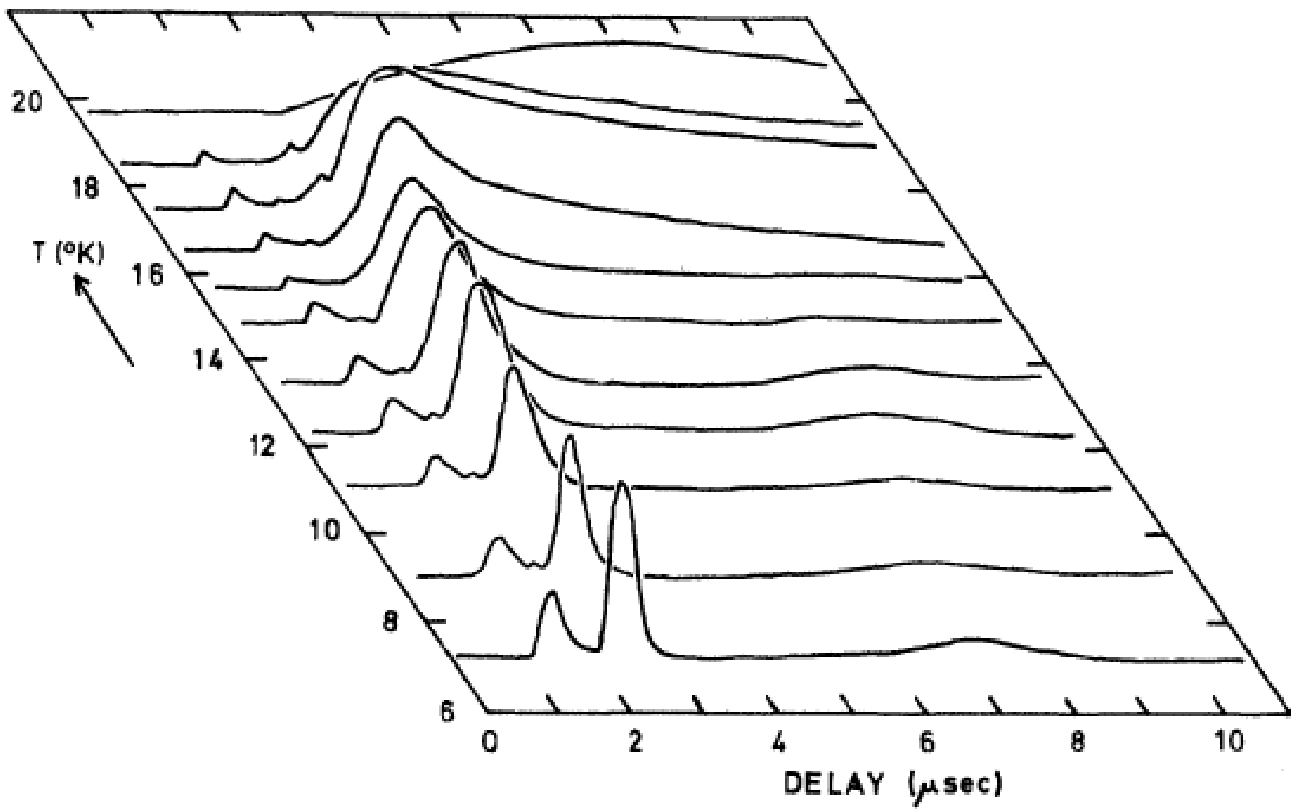
$$\mu_g = \frac{1}{3} e \tau_N, \quad \zeta_g = \frac{\tau e (1 - c_2^2 / c_1^2)}{(1 - i\omega\tau)}, \quad \tau^{-1} = \tau_N^{-1} + \tau_R^{-1}$$

μ_g: the first viscosity, ζ_g: the second viscosity

Rogers, Physical Review B, Vol. 37, p1440-1457, 1971

Numerical Reconstruction of Heat-Pulse Experiments





McNelly, PhD. Thesis, 1974

Rogers, Physical Review B, Vol. 37, p1440-1457, 1971

Hybrid Phonon Gas Model (Mixture of Longitudinal & Transverse Phonons)

- **Mixture theory of longitudinal and Transversal phonons in <100> crystallographic direction:**

$$E = E_l + 2E_t, \quad \vec{q} = \vec{q}_l + 2\vec{q}_t$$

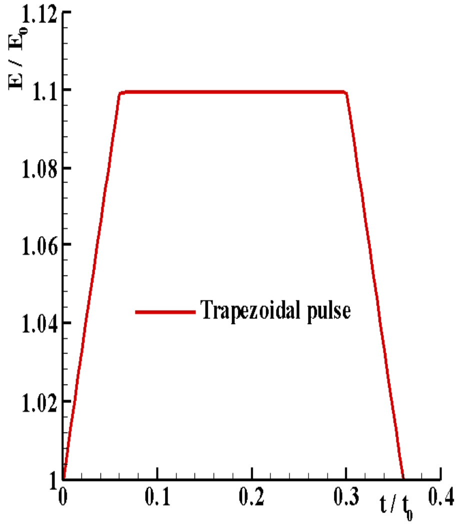
- **Dispersion relationship of of longitudinal phonons (gray model):**

$$k_{lr} = \frac{\omega}{c_l}, \quad k_{li} = \left(\frac{1}{3\tau_N} + \frac{5}{6\tau_R} \right) \frac{1}{c_l}$$

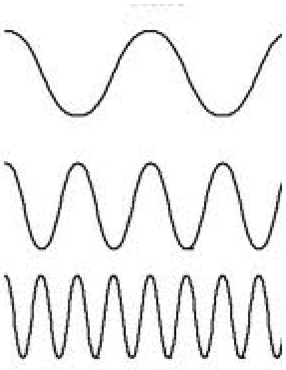
- **Dispersion relationship of transversal phonons (Rogers'model):**

$$\frac{1}{3} k_t^2 = \omega^2 \frac{1 + \frac{\tau}{\tau_R} - i\left(\omega\tau - \frac{1}{\omega\tau_R} \right)}{1 - 3i\omega\tau}$$

Numerical Methods



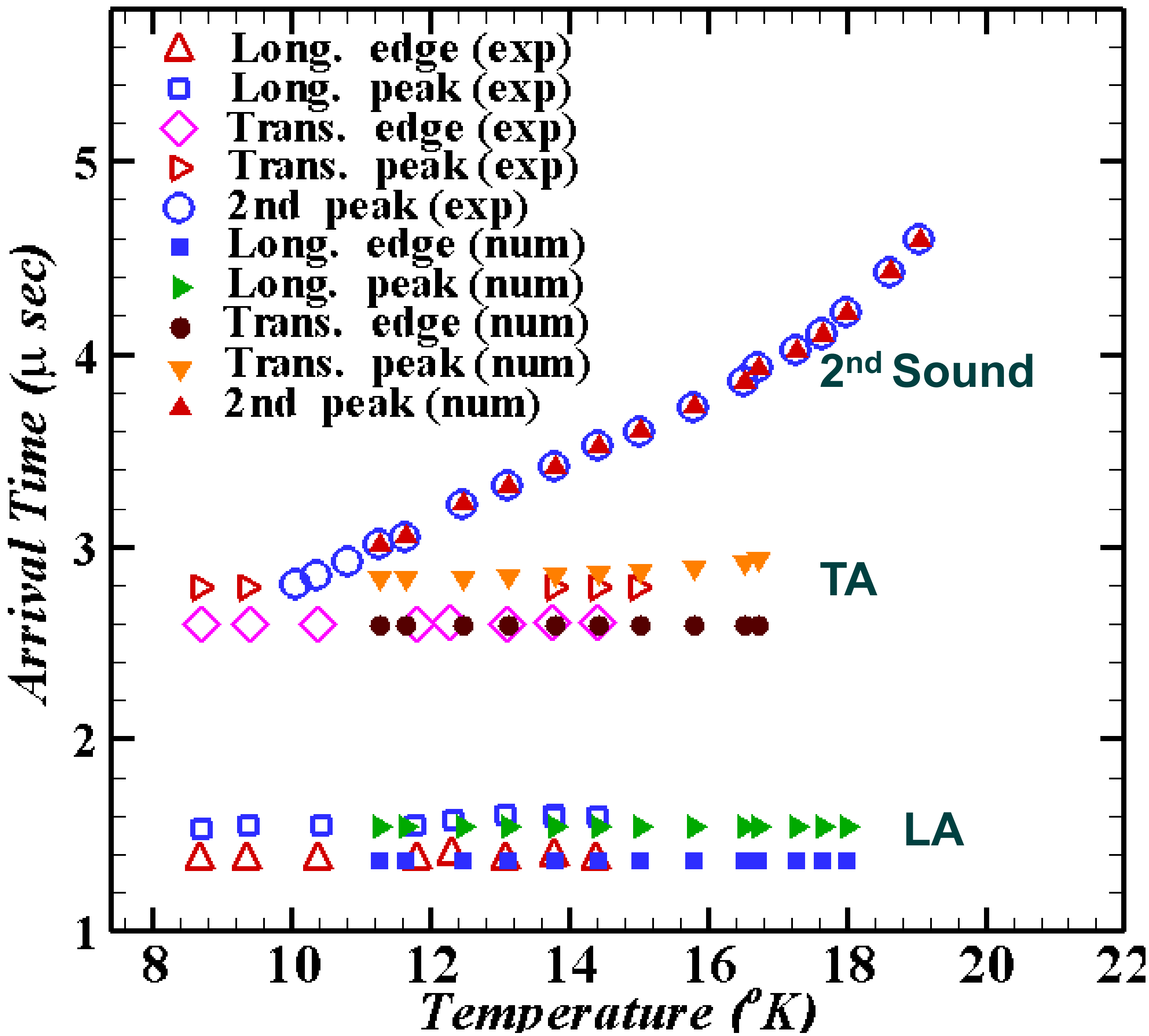
$$= \sum$$



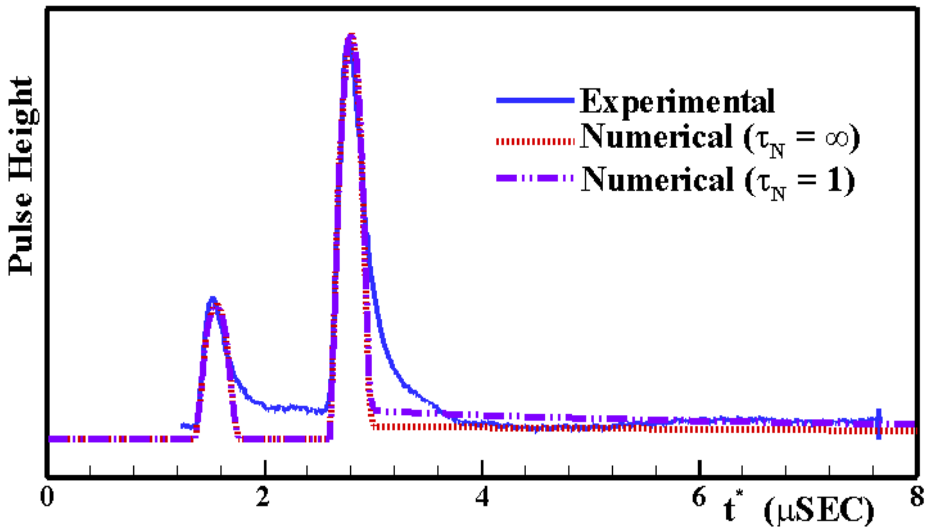
$$f(0,t) = \sum_{j=0}^{\infty} b_j e^{i(-\omega_j t)}$$

$$f(x,t) = \sum_{j=0}^{\infty} b_j e^{i(k_j x - \omega_j t)}$$

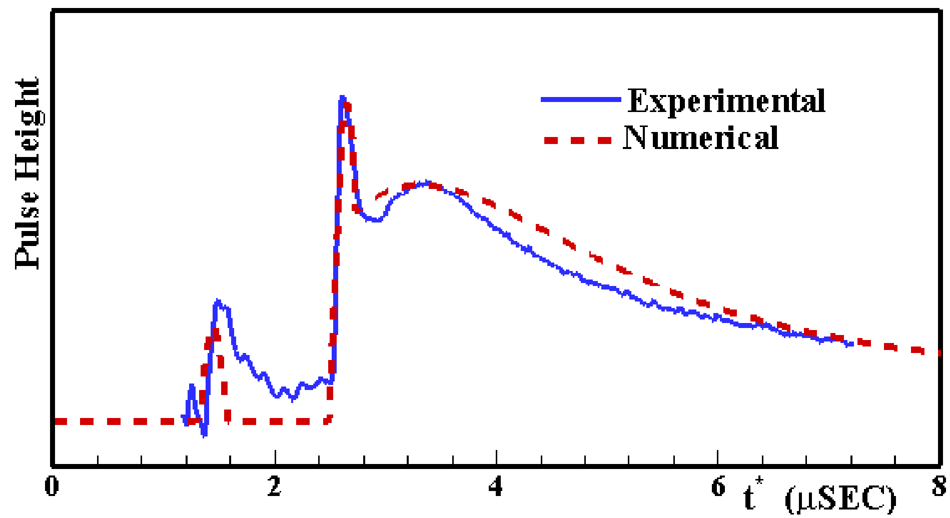
Comparison of Arrival Time of Heat Pulses in Very Pure NaF



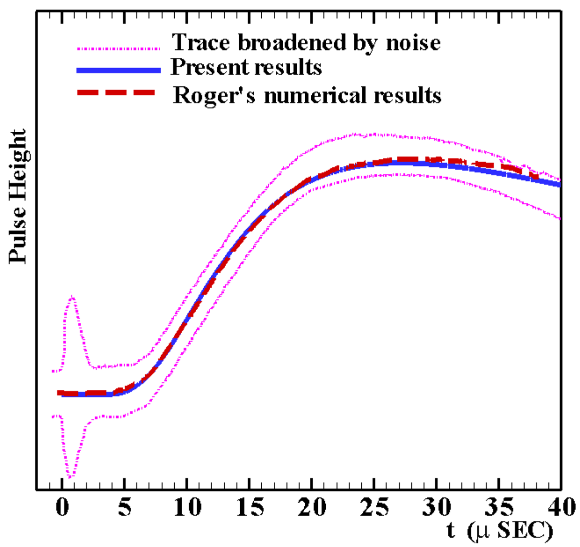
Reconstruction of Heat-Pulse Experiments in Pure NaF

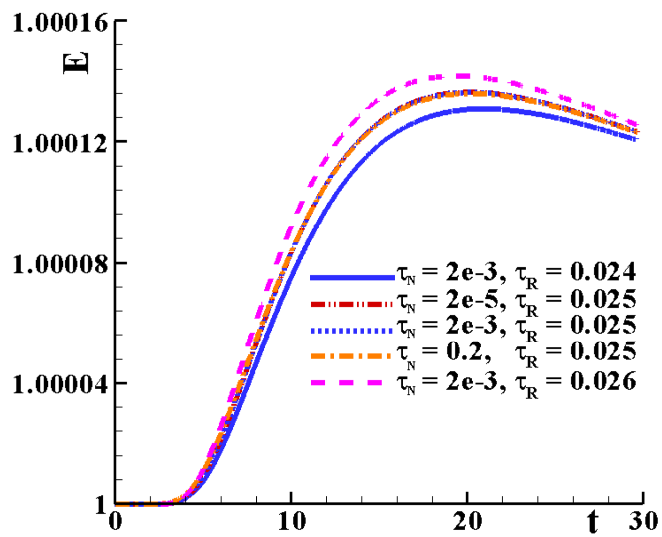


Comparison of detected heat pulses at x = 1, T^* = 9.6K.



Comparison of detected heat pulses at x = 1, T^* = 13K.





Comparison of detected heat pulses at x = 1, T^* = 25.5K.

Journal paper under review

Non-Fourier Heat Conduction Models

- **Energy equation:** $\frac{\partial e}{\partial t} + \nabla \cdot \vec{q} = 0$
- **Evolution equation for heat flux:**

1. **Fourier's Law:** $\vec{q} = -k\nabla T$

   (Infinite speed of propagation & fail for ballistic phonons)

2. **Cattaneo-Vernotte model:** $\tau_R \frac{\partial \vec{q}}{\partial t} + \vec{q} = -k\nabla T$

   (Allow 2nd sound propagation but fail for ballistic phonons)

3. **Guyer-Krumhansl model:**

$$\frac{\partial \vec{q}}{\partial t} + \frac{\vec{q}}{\tau_R} = -\frac{k}{\tau_R}\nabla T + \frac{k\tau_N}{5}\left(\nabla^2 \vec{q} + 2\nabla(\nabla \cdot \vec{q})\right)$$

   (Prediction of second sound: $\tau_N \ll \tau_R$, fail for ballistic phonons)

Non-Fourier Heat Conduction Model Based on Fractional Derivative ?

1. **Fourier's Law:** $\vec{q} = -k\nabla T$
2. **Fractional derivative for Non-Fourier's heat conduction model:**

$$\vec{q} = -k\nabla^{a} T \;?$$

$$\frac{\partial^{\xi}\vec{q}}{\partial t^{\xi}} + \frac{\vec{q}}{\tau_R} = -\frac{k}{\tau_R}\nabla T + \beta(\nabla^{\eta}\vec{q}) \quad ?$$

Summary

- A Ballistic-Diffusive Phonon Hydrodynamic (BDPH) model was developed for ballistic-diffusive phonon transport.
- The model is validated by comparing against heat pulse experiments.
- Seek the possibility of developing non-Fourier heat conduction model based on fractional calculus.

Thank you!