Internal variables and heat conduction in non-equilibrium thermodynamics

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Dec 7. 2015.

About the non-relativistic heat conduction

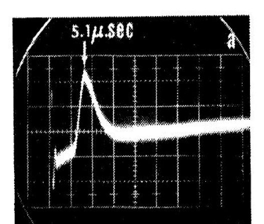
- Paradox of the Fourier equation: infinite speed of propagation, parabolic type equation ("a": thermal diffusivity)

$$\partial_t T = a\partial_{xx} T$$

- First modification (1958): Maxwell-Cattaneo-Vernotte (MCV) equation $\rightarrow$ hyperbolic type, finite propagation speed $\rightarrow$ second sound, temperature: around 1-20 K

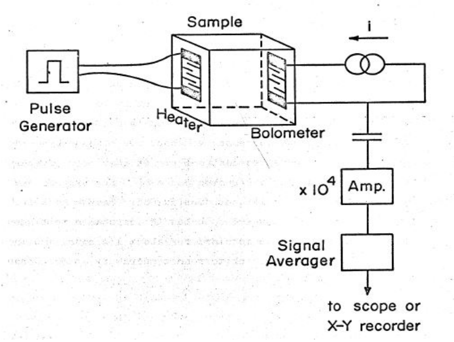
$$\tau_q \partial_{tt} T + \partial_t T = a\partial_{xx} T$$

Narayanamurti et al.: Experimental proof of second sound in Bi ('74)



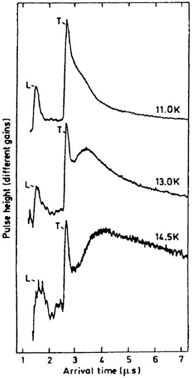
Experiments I.

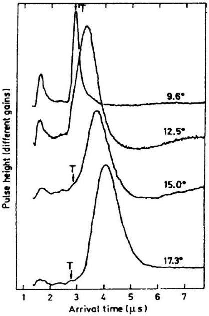
What is the heat pulse experiment?!



Experiments II.

Beyond the phenomena of second sound $\rightarrow$ ballistic propagation





Jackson - Walker - McNelly experiments on NaF material (1968-70).
The 3 propagation types can be clearly distinguished!

How can it be modeled?
Kinetic theory + RET: phonon hydrodynamics

Kinetic theory - phonon hydrodynamics I.

Interactions $\rightarrow$ distributions

- Normal (N) processes: momentum is conserved
- Resistive (R) processes: momentum is not conserved
- Umklapp-processes: neither the energy, nor the momentum is conserved

Connection to heat conduction

- R-processes are dominant: diffusive propagation (Fourier)
- N-processes are dominant: wave propagation (MCV...)
- Ballistic propagation: heat conduction without interactions!

Kinetic theory - phonon hydrodynamics II.

Momentum series expansion + truncation closure

$$u_{\langle i_1 i_2 \dots i_N \rangle} = \int k n_{\langle i_1 \dots i_n \rangle} f dk.$$

$$\frac{\partial u_{\langle n \rangle}}{\partial t} + \frac{n^2}{4n^2-1} c \frac{\partial u_{\langle n-1 \rangle}}{\partial x} + c \frac{\partial u_{\langle n+1 \rangle}}{\partial x} = \begin{cases} 0 & n = 0 \\ -\frac{1}{\tau_R} u_{\langle 1 \rangle} & n = 1 \\ -\left(\frac{1}{\tau_R} + \frac{1}{\tau_N}\right) u_{\langle n \rangle} & 2 \leq n \leq N \end{cases}$$

It requires at least N=30 momentum equation to obtain the real propagation speeds.
Results? See later!

About the internal variables

- Non-equilibrium description
- Nonlocal extensions in space and time → generalizations
  - Rheology: Kluitenberg-Verhas body
  - Dual internal variables: beyond the Newton equation
  - Wave propagation: coupling between mechanical and thermal effects
- Non-equilibrium thermodynamics → heat conduction
  - Diffusive propagation → Fourier
  - Wave propagation ("Second sound') → Maxwell-Cattaneo-Vernotte, Guyer-Krumhansl, and so on...
  - Ballistic propagation → An unified continuum theory is missing! Propagation with speed of sound, mechanical coupling!

Continuum theory - Generalization of heat conduction I

Tensorial internal variable + extended entropy current:

- q^i is a *basic field variable*; Q^{ij} is an *internal variable*
- entropy density: $s(e, q^i, Q^{ij}) = s_e(e) - \frac{m_1}{2} q^i \cdot q^i - \frac{m_2}{2} Q^{ij} \cdot Q^{ij}$
- entropy current: $J^i = b^{ij} q^j + B^{ijk} Q^{jk}$

Entropy production in 1 spatial dimension:

$$\left(b - \frac{1}{T}\right) \partial_x q + (\partial_x b - m_1 \partial_t q)\, q - (\partial_x B - m_2 \partial_t Q)\, Q + B \partial_x Q \geq 0$$

Linear relations between *thermodynamic fluxes* and *forces*, isotropy:

$$\begin{aligned} m_1 \partial_t q - \partial_x b &= -l_1 q, \\ m_2 \partial_t Q - \partial_x B &= -k_1 Q + k_{12} \partial_x q, \\ b - \frac{1}{T} &= -k_{21} Q + k_2 \partial_x q, \\ B &= n \partial_x Q. \end{aligned}$$

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B &= \cancel{n \partial_x Q}.
\end{aligned}$$

Compatibility with kinetic theory

Properties of the hierarchical structure

- New quantity: $Q^{ij} \rightarrow$ flux of the heat flux
- Effective model in the sense of material parameters
- Incorporates the *ballistic* effect
- Hyperbolic system:
  - finite propagation speeds
  - the existence and uniqueness of the solution is proved

Generalized (dimensionless) equations

- MCV: $\tau_q \partial_{tt} T + \partial_t T = \partial_{xx} T$
- GK: $\tau_q \partial_{tt} T + \partial_t T = \partial_{xx} T + \kappa^2 \partial_{txx} T$
- Green-Naghdi: $\tau_q \partial_{tt} T = \partial_{xx} T + \kappa^2 \partial_{txx} T$
- Ballistic-conductive:
  $\tau_q \tau_Q \partial_{ttt} T + (\tau_q + \tau_Q) \partial_{tt} T + \partial_t T = \partial_{xx} T + (\kappa^2 + \tau_Q) \partial_{txx} T$

Hierarchy: Guyer-Krumhansl equation

With eliminated heat flux:

$$\tau_q \partial_{tt} T + \partial_t T = \partial_{xx} T + \kappa^2 \partial_{txx} T$$

Fourier equation:

$$\tau_q \partial_{tt} T + \partial_t T = \partial_{xx} T + \kappa^2 \partial_{txx} T$$

Time derivative of the Fourier equation: $\tau_q = \kappa^2$

$$\tau_q \partial_{tt} T + \partial_t T = \partial_{xx} T + \kappa^2 \partial_{txx} T$$

Solutions when $\tau_q \neq \kappa^2$? See after the experiments!
Further example: rheology - hierarchy of the Hooke body...

Heat pulse experiments III. - NaF samples

Well-documented series of experiments...but

- The samples can be hardly distinguished (by peak thermal conductivity and sample length)
- The boundary conditions are not clear (e.g. pulse length)
- The fitted and measured material parameters $\rightarrow$ temperature dependency?!
- Cooling effect during propagation? (see the fitting...)
- Can it be simulated as 1+1D problem? (longitudinal and transverse modes, excitation...)

The ballistic-conductive model I.

System of equations in *dimensionless* form:

$$
\begin{aligned}
\tau_\Delta \frac{\partial T}{\partial t} + \frac{\partial q}{\partial x} &= 0, \\
\tau_q \frac{\partial q}{\partial t} + q + \tau_\Delta \frac{\partial T}{\partial x} + \kappa \frac{\partial Q}{\partial x} &= 0, \\
\tau_Q \frac{\partial Q}{\partial t} + Q + \kappa \frac{\partial q}{\partial x} &= 0.
\end{aligned}
$$

Finite difference discretization

- Explicit scheme $\rightarrow$ stability conditions with von Neumann method and Jury criterion.

The ballistic-conductive model II. - IC&BC

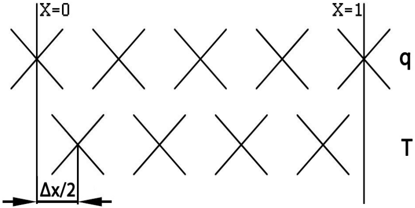
Initial conditions

All fields are zero at t=0.

Boundary conditions

Only for the field of heat flux → *discretization* method!

$$q(t, x=0) = \begin{cases} 1 - cos(2\pi \cdot \frac{t}{t_{impulse}}) & \text{if } 0 < t \leq t_{impulse} \\ 0 & \text{if } t > t_{impulse} \end{cases}$$



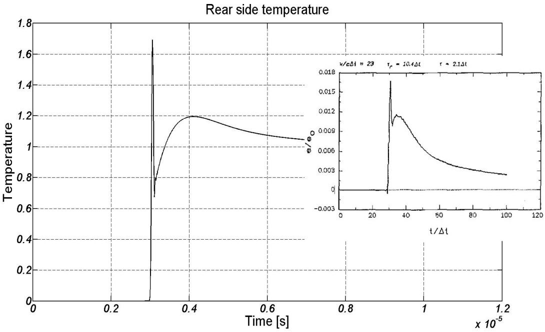
Shifted fields:
One goes from $x = 0$ to $x = 1$, the others shifted by $\frac{\Delta x}{2}$.

The ballistic-conductive vs. RET (Dreyer-Struchtrup)

Material parameters: $k = 13500\frac{W}{mK}, c = 1.8\frac{J}{kgK}, \rho = 2866\frac{kg}{m^3}$

Other parameters:

$$L = 6.3mm, \Delta t = 10^-7s, \tau_q = 10.4\Delta t, \tau_Q = 2.1\Delta t$$



Adiabatic boundary condition?!

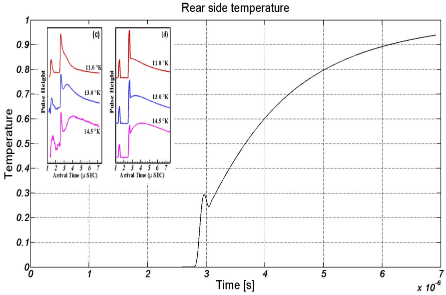
The ballistic-conductive model vs. Y. Ma model

Complex viscosity model (Landau, Rogers...)

Material parameters: $k = 13500\frac{W}{mK}, c = 1.8\frac{J}{kgK}, \rho = 2866\frac{kg}{m^3}$

Other parameters:

$$L = 7.9mm, \Delta t = 0.24\mu s, \tau_q = 0.937\mu s, \tau_Q = 0.248\mu s$$



Adiabatic boundary condition?! Modify the balance equation!

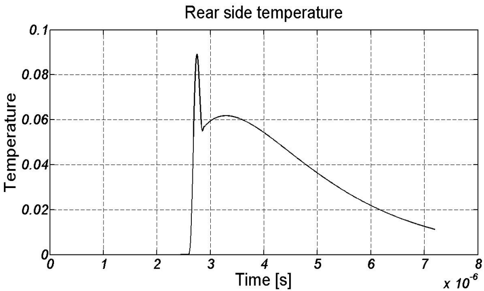
The ballistic-conductive model - Solution

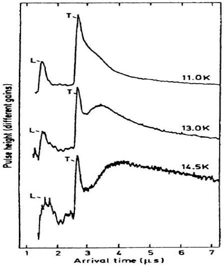
$$\partial_t e + \nabla \cdot \mathbf{q} = -\alpha(T_{wave} - T_0),$$

Material parameters:

$$k = 10200\frac{W}{mK}, c = 1.8\frac{J}{kgK}, \rho = 2866\frac{kg}{m^3}$$

$$\tau_q = 0.355\mu s, \tau_Q = 0.21\mu s \text{ and } L = 7.9mm, \Delta t = 0.24\mu s$$

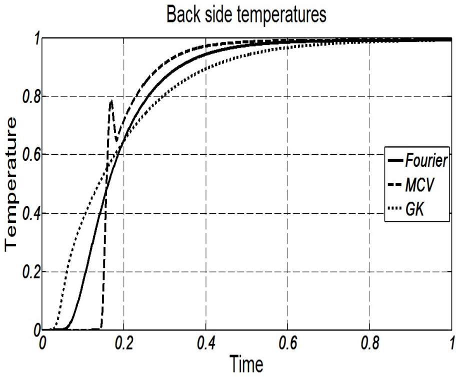




The ballistic-conductive model - further solutions I.

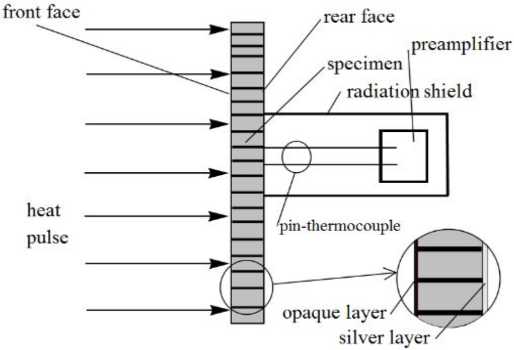
Guyer-Krumhansl equation:

$$\tau_q \partial_{tt} T + \partial_t T = \partial_{xx} T + \kappa^2 \partial_{txx} T$$



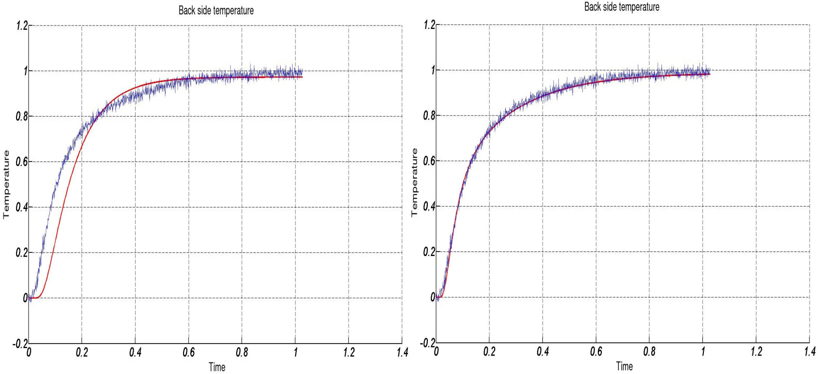
Non-Fourier solutions...
MCV-region: $\tau_q > \kappa^2$
GK-region: $\tau_q < \kappa^2$
On room temperature?!
Inhomogeneity...
EXPERIMENT!

The ballistic-conductive model - further solutions II.



Arrangement of the measurement

The ballistic-conductive model - further solutions III.



Measurement on room temperature, layered sample
On macroscopic scale the GK equation is the relevant generalization to characterize non-Fourier heat conduction.

Thank you for your kind attention!