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# Finite Element Analysis of Transient Ballistic-Diffusive Heat Transfer in Two-Dimensional Structures



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### Motivation

- Size of electronic devices gets smaller and smaller such as in CPUs and transistors
- Sub-continuum heat conduction is important
- Different numerical works have been done in modeling ballistic-diffusive heat transfer
- Not available for public in any commercial package



An SEM image of an upright-type double-gate MOS transistor (Source: AIST)



Singh et al. J. of Heat Transfer, 2011



### Heat transfer equations

Fourier equation

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

- Continuum medium
- Diffusive thermal transport (Parabolic equation)
- Cannot accurately predict sub-continuum heat transfer

- Boltzmann transport equation (BTE)
  - Based on energy carriers distribution (statistical base)
  - Complicated scattering term
  - Relaxation time approximation

$$\frac{\partial f}{\partial t} + \mathbf{v}_g \cdot \nabla f = \frac{f_0 - f}{\tau}$$

- f frequency dependent distribution function
- $\mathbf{v}_{g}$  group velocity of energy carriers
  - $f_0$  equilibrium distribution function
- au effective relaxation time



### **Governing equation**

BTE for phonon energy density

$$\frac{\partial e''}{\partial t} + \nabla \cdot (v_g \hat{\mathbf{s}} e'') = \frac{e_0'' - e''}{\tau}$$

$$e''(\mathbf{r}, \hat{\mathbf{s}}, t) = \sum_{p} \left( \int_{0}^{\omega_{p}} D_{p}(\omega) f \hbar \omega d\omega \right)$$
Directional phonon energy density  
$$e''_{0}(\mathbf{r}, t) = \frac{1}{4\pi} \int_{4\pi} e''(\mathbf{r}, \hat{\mathbf{s}}, t) d\Omega$$
Equilibrium phonon energy density

 $v_{g}$  Phonon group velocity

### Knudsen number $Kn = \Lambda / L$

For a constant phonon mean free path: Smaller domain length ightarrow Larger Kn



#### Nondimensional 2-D BTE + DOM

$$\frac{1}{\mathrm{Kn}} \frac{\partial e_{n,m}''}{\partial t^*} + \mu_n \frac{\partial e_{n,m}''}{\partial x^*} + \eta_{n,m} \frac{\partial e_{n,m}''}{\partial y^*} = \frac{e_0'' - e_{n,m}''}{\mathrm{Kn}}$$
$$\mu_n = \cos \theta_n \qquad t^* = t/\tau$$
$$\pi_{n,m} = \sin \theta_n \cos \varphi_m \qquad y^* = y/\mathrm{H}$$



#### **Discrete Ordinate Method (DOM)**

$$e_0''(\mathbf{r},t) = \frac{1}{4\pi} \int_{4\pi} e''(\mathbf{r},\hat{\mathbf{s}},t) d\Omega$$
$$e_0''(t^*, x^*, y^*) = \frac{2}{4\pi} \sum_n \sum_m e_{n,m}''(t^*, x^*, y^*) w_n w_m'$$





### Validation (1-D thin film)



[1] G. Chen, Nanoscale Energy Transport and Conversion,Oxford University Press, 2005.



#### Results





## Ray effect



Diffusive



#### **Transient solution**



- COMSOL can calculate sub-continuum phonon heat transport.
- FEA-DOM combination is used in COMSOL for ballistic-diffusive heat transfer.
- Modeling nanoscale heat transfer is easily accessible.

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#### Recently accepted in: International Journal of Heat and Mass Transfer

Doi: 10.1016/j.ijheatmasstransfer.2014.09.073





### Introduction

Application:

Thermomechanical data writing/reading Thermal performance of extremely miniaturized electronic devices Thermal etching Thermal deposition



Pires et al., Science., 328 (2010)



Lee et al., Nano Lett., 10 (2010)



### Heat transfer equations

• Fourier equation

Energy conservation + Fourier's heat flux approximation Used for heat conduction simulation for the last 2 centuries Heat carriers travel with an infinite speed

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

Hyperbolic wave equation

$$\frac{1}{C^2} \frac{\partial^2 u}{\partial t^2} = \nabla^2 u$$

• Hyperbolic heat equation (Cattaneo equation) Finite speed of heat carriers  $C^2 = \frac{\alpha}{\tau}$ Good for short time scales but not for short spatial scale

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \alpha \nabla^2 T$$



### Fourier and hyperbolic heat equations

Joshi and Majumdar, Journal of Applied Physics, 1993



Transient Fourier and Hyperbolic heat equation

Steady state Fourier and Hyperbolic heat equation



### **Boltzmann Transport Equation (BTE)**

• Boltzmann transport equation (BTE)

BTE has a statistical base based on energy carriers distribution

$$\frac{\partial f}{\partial t} + \mathbf{v}_g \cdot \nabla f = \left[\frac{\partial f}{\partial t}\right]_{scattering}$$

- f frequency dependent distribution function
- $\mathbf{v}_{g}$  group velocity of energy carriers (phonons)

• Relaxation time approximation

$$\left[\frac{\partial f}{\partial t}\right]_{scattering} = \frac{f_0 - f}{\tau}$$

- $f_0$  equilibrium Bose-Einstein distribution
- au effective relaxation time

$$e_0''(t^*, x^*, y^*) = \frac{2}{4\pi} \sum_n \sum_m e_{n,m}''(t^*, x^*, y^*) w_n w_m'$$

$$\sum_{n}\sum_{m}w_{n}w_{m}'=2\pi$$

$$T(t^*, x^*, y^*) = \frac{4\pi e_0''(t^*, x^*, y^*)}{C} = \frac{2}{C} \sum_n \sum_m e_{n,m}''(t^*, x^*, y^*) w_n w_m'$$

$$q_x''(t^*, x^*, y^*) = 2v_g \sum_n \sum_m e_{n,m}''(t^*, x^*, y^*) \mu_n w_n w_m'$$
$$q_y''(t^*, x^*, y^*) = 2v_g \sum_n \sum_m e_{n,m}''(t^*, x^*, y^*) \eta_{n,m} w_n w_m'$$

$$e''(\mathbf{r}_b, \mathbf{s}) = e_0''(\mathbf{r}_b) = \frac{CT_b}{4\pi}$$



### **COMSOL** model



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## Ray effect





#### COMSOL model

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DE 6 (c6)	$e_{a}\frac{\partial u}{\partial t^{2}} + d_{a}\frac{\partial u}{\partial t} + \nabla \cdot (-c\nabla u - \alpha u + \gamma) + \beta \cdot \nabla u + au = f$	0.2
▷ Δ <sub>U</sub> PDE 7 (c7)	$\nabla = \left[\frac{\partial}{\partial t}, \frac{\partial}{\partial t}\right]$	
DE 8 (c8)	· dx'dy'	0.1
∆u PDE 9 (c9)	▼ Diffusion Coefficient	
D ∆u PDE 10 (c10)		
▷ ∆u PDE 11 (c11)		-0.1
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ν Δυ PDE 13 (C13)	Isotropic	-0.2
Au PDE 15 (c15)		
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▷ Δυ PDE 20 (c20)	▼ Source Term	
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DE 22 (c22)	f (0.007*(0.1590*u+0.3493*u2+0.4928*u3+0.5697*u4+0.5697*u5+0.4928*u6+0.3493*u7+) 1/m <sup>2</sup>	-0.7
Au PDE 23 (c23)		
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