6th INTERNATIONAL WORKSHOP ON NON-EQUILIBRIUM THERMODYNAMICS
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GENERALIZED TRANSPORT EQUATIONS FOR HEAT TRANSFER IN NANOSYSTEMS

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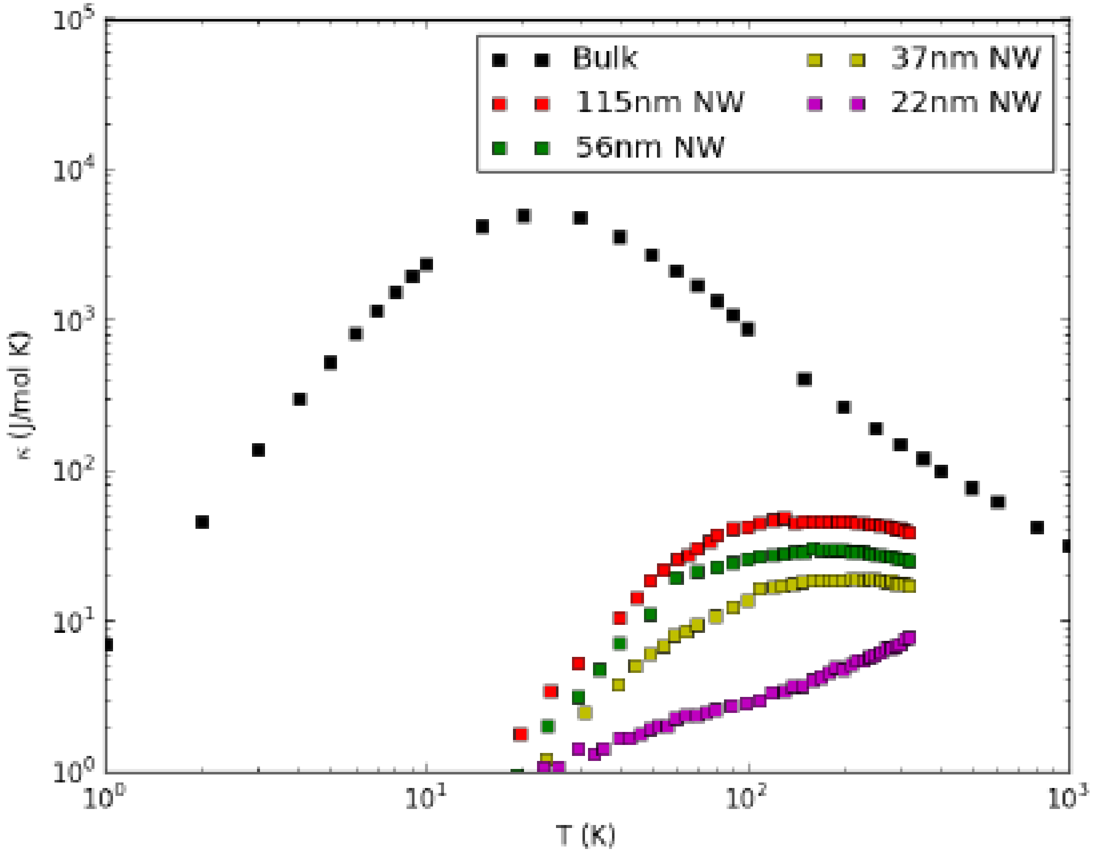
PLAN

- Generalized heat transport equations incorporating non-vanishing collision time and mean-free path

- nanowires (silicon nanowires and metallic nanowires, size-dependent thermal conductivity)
- plane sheets (silicon layers and graphene sheets, radial heat transfer from a central heat source).

- a) influence of boundary conditions (smooth or rough walls);
- b) phonon and electron heat transfer in metallic nanowires;
- c) compatibility with the second law;
- d) thermal wave propagation.

SIZE DEPENDENCE OF HEAT CONDUCTIVITY



ELEMENTARY KINETIC THEORY

- Mean free path $\kappa = \frac{1}{3}\rho \mathbf{c}\mathbf{v}\ell = \frac{1}{3}\rho \mathbf{c}\mathbf{v}^2\tau$, $\kappa = \int \hbar\omega \vec{v}_g \, \tau \frac{\partial f}{\partial T} D(\omega) d\omega$
- Collision time

$$\frac{1}{\tau} = \frac{1}{\tau_{\mathbf{bulk}}} + \frac{1}{\tau_{\mathbf{wall}}}$$

- Heat conductivity

$$\kappa = \frac{\kappa_0}{1 + \frac{\tau_{\mathbf{b}}}{\tau_{\mathbf{w}}}} = \frac{\kappa_0}{1 + \alpha \frac{\ell}{R}}$$

- Limiting behaviours $\ell << R \rightarrow \kappa = \kappa_0 ;\ \ell >> R \rightarrow \kappa = \kappa_0 (R/\alpha\ell)$
- Heat conductivity

$$\kappa = \kappa\left(T; \frac{\ell}{R}; \frac{\ell_q}{R}; R\nabla \ln T \right)$$

- Walls, quantum localization, nonlinear

KINETIC THEORY

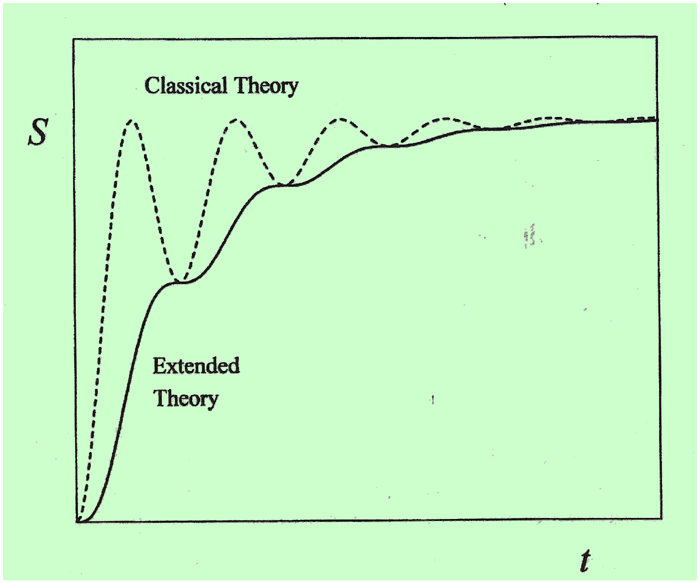
- Relaxation time approximation $$\frac{\partial f}{\partial t} + c \cdot \nabla f = -\frac{f - f_0}{\tau}$$
- Solution
$$f = \frac{1}{1 + \boldsymbol{\tau c} \cdot \nabla} f_0 = f_0 - \tau c \cdot \nabla f_0 + \frac{1}{2}\tau^2 c^2 \nabla^2 f_0$$
- Two possibilities
- Heat flux a $$\boldsymbol{q} = -\kappa_0 \nabla T + \ell^2 \nabla^2 \boldsymbol{q}$$
- Heat flux b $$\boldsymbol{q} = -\frac{\kappa_0}{1 + \alpha \frac{\ell}{R}} \nabla \boldsymbol{T} + \frac{\ell^2}{\left(1 + \alpha \frac{\ell}{R}\right)^2} \nabla^2 \boldsymbol{q}$$

TRANSPORT EQUATIONS AND SECOND LAW

- Current technology requires generalized transport equations with memory and nonlocal effects, e.g.
-
  - $$\tau \frac{\partial \boldsymbol{q}}{\partial t} = -(\boldsymbol{q} + \lambda \nabla T) + \ell^2 \nabla^2 \boldsymbol{q}$$
  - This describes experiments but is not compatible with local equilibrium, entropy and entropy flux must be generalized

$$s(u, \boldsymbol{q}) = s_{eq}(u) - \frac{\tau}{2\rho\lambda T^2} \boldsymbol{q} \cdot \boldsymbol{q}$$

$$\boldsymbol{J}^s = \frac{1}{T}\boldsymbol{q} - \frac{\ell^2}{\lambda T^2}(\nabla \boldsymbol{q}) \cdot \boldsymbol{q}$$

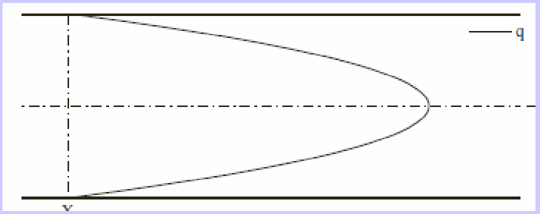


NONLOCAL HEAT TRANSPORT WITH RELAXATION: PHONON HYDRODYNAMICS

$$\tau\dot{\mathbf{q}} + \mathbf{q} = -\kappa_0 \nabla T + l^2 \nabla^2 \mathbf{q}.$$

$$\nabla^2 \mathbf{q} = \frac{\kappa_0}{l^2} \nabla T.$$

$$\nabla^2 \mathbf{v} = \frac{1}{\eta} \nabla p$$



$$V_P(r) = \frac{\Delta p}{4L\eta}[R^2 - r^2]$$

$$Q = \frac{\pi R^4}{8\eta} \frac{\Delta p}{L}$$

$$Q^{(h)} = \frac{\pi R^4 \kappa_0}{8 l^2} \frac{\Delta T}{L}$$

$$\kappa_{\text{eff}}^{(\text{nw})}\left(\frac{l}{R}\right) = \frac{Q^{(h)}}{\pi R^2} \frac{L}{\Delta T} = \frac{\kappa_0}{8} \frac{R^2}{l^2}$$

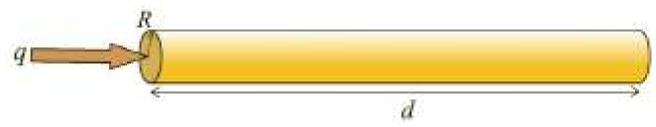
$$V_{\text{surf}} = Cl\left(\frac{\partial V_P}{\partial r}\right)_{r=R}$$

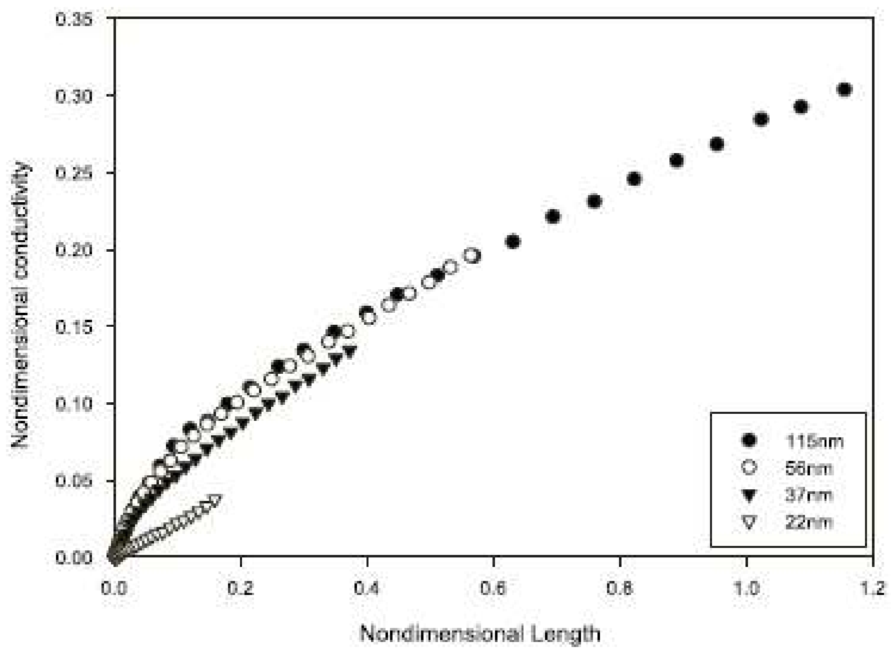
$$\kappa_{\text{eff}}^{(\text{nw})}\left(\frac{l}{R}\right) = \frac{Q^{(h)}}{\pi R^2} \frac{L}{\Delta T} = \frac{\kappa_0}{8} \frac{R^2}{l^2}\left[1 + 4C\frac{l}{R}\right]$$

PHONON HYDRODYNAMICS AND HEAT TRANSPORT IN NANOWIRES

$$\tau\dot{\mathbf{q}} + \mathbf{q} = -\kappa_0 \nabla T + l^2 \nabla^2 \mathbf{q}.$$

$$\kappa_{\text{eff}}^{(\text{nw})}\left(\frac{l}{R}\right) = \frac{Q^{(h)}}{\pi R^2}\frac{L}{\Delta T} = \frac{\kappa_0}{8}\frac{R^2}{l^2}\left[1 + 4C\frac{l}{R}\right]$$

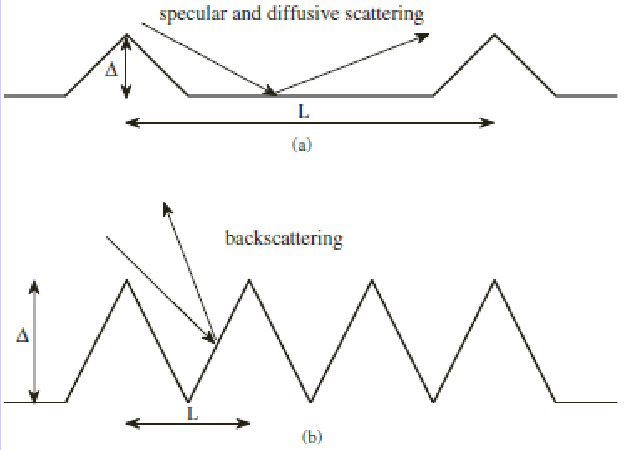




THERMAL CONDUCTIVITY OF SMOOTH AND ROUGH NANOWIRES

$$q_w(r) = Cl\left(\frac{\partial q_b}{\partial r}\right)_{r=d} - \alpha l^2\left(\frac{\partial^2 q_b}{\partial r^2}\right)_{r=d}$$

$$\kappa_{eff} = \frac{\kappa_0}{8\ \mathrm{Kn}^2}(1 + 4C\ \mathrm{Kn} - 4\alpha\ \mathrm{Kn}^2)$$



$$C = C'\left(1 - \frac{\Delta}{L}\right)$$

$$\alpha = \alpha'\frac{\Delta}{L},$$

TABLE I. Bulk thermal conductivity κ_0 and mean-free path l of phonons in silicon nanowires for different values of temperature. These values are taken from experimental data.[29]

	$T=150$ K	$T=100$ K	$T=80$ K	$T=60$ K	$T=50$ K	$T=40$ K	$T=30$ K
κ_0 (W/mK)	409	884	1340	2110	2680	3530	4810
l (nm)	181	557	1432	3837	6681	11517	16354

THERMAL CONDUCTIVITY OF SMOOTH NANOWIRES

TABLE II. Experimental values of the effective thermal conductivity in silicon nanowires with different radii R and at several values of temperature in the absence of backscattering ($\Delta=0$ nm). The experimental data have been inferred from Ref. 29.

	$T=150$ K	$T=100$ K	$T=80$ K	$T=60$ K	$T=50$ K	$T=40$ K	$T=30$ K
R (nm)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)
115	46	45	40	27	19	13	5
56	28	23	21	16	11	7	3
37	17	14	11	8	6	4	1.7

TABLE IV. Theoretical predictions for the value of the effective thermal conductivity in silicon nanowires with different radii R and at several values of temperature in the absence of backscattering ($\Delta=0$ nm). The values are obtained by using the model described by Eqs. (5), (6a), (6b), and (7).

	$T=150$ K	$T=100$ K	$T=80$ K	$T=60$ K	$T=50$ K	$T=40$ K	$T=30$ K
R (nm)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)
115	68.3	45.5	40.3	27.6	19.0	11.7	6.4
56	28.1	20.9	19.4	13.4	9.2	5.7	3.1
37	17.5	13.6	12.7	8.8	6.1	3.8	2.1

THERMAL CONDUCTIVITY OF ROUGH NANOWIRES

TABLE III. Experimental values of the effective thermal conductivity in silicon nanowires with different radii R and at several values of temperature in the presence of backscattering ($\Delta=3$ nm and $L=6$ nm). The experimental data have been inferred from Refs. 14 and 15.

	$T=150$ K	$T=100$ K	$T=80$ K	$T=60$ K	$T=50$ K	$T=40$ K	$T=30$ K
R (nm)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)
115	7.8	5.7	4.9	3.3	2.5	1.8	1.3
97	5.3	3.8	3.2	2.1	1.7	1.2	0.9

TABLE V. Theoretical predictions for the value of the effective thermal conductivity in silicon nanowires with different radii R and at several values of temperature in the presence of backscattering ($\Delta=3$ nm and $L=6$ nm). The values are obtained by using the model described by Eqs. (5), (6a), (6b), and (7).

	$T=150$ K	$T=100$ K	$T=80$ K	$T=60$ K	$T=50$ K	$T=40$ K	$T=30$ K
R (nm)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)	κ_{eff} (W/mK)
115	15.1	6.9	6.5	4.2	2.3	1.3	2.0
97	5.4	2.4	3.1	2.0	0.8	0.4	1.5

THERMAL AND ELECTRICAL CONDUCTIVITY IN METALLIC NANOWIRES. WIEDEMANN-FRANZ

$$\tau_e \dot{q}_i^{(e)} + q_i^{(e)} = -\kappa_e \theta_{,i} + \ell_e^2 \left(q_{i,jj}^{(e)} + 2 q_{j,ji}^{(e)} \right),$$
$$\tau_p \dot{q}_i^{(p)} + q_i^{(p)} = -\kappa_p \theta_{,i} + \ell_p^2 \left(q_{i,jj}^{(p)} + 2 q_{j,ji}^{(p)} \right),$$

$$\tau_E \dot{J}_i + J_i = \sigma E_i + \ell_E^2 \left(J_{i,jj} + 2 J_{j,ji} \right),$$

$$\kappa_e^{eff} = C_e \frac{\kappa_e}{2} \frac{R}{\ell_e},$$
$$\kappa_p^{eff} = C_p \frac{\kappa_p}{2} \frac{R}{\ell_p},$$
$$\sigma^{eff} = C_E \frac{\sigma}{2} \frac{R}{\ell_E}.$$

THERMAL CONDUCTIVITY OF POROUS SI

$$\kappa_{eff} = f(\phi)\kappa_0$$

$$f(\phi) = (1-\phi)^3$$

$$F = \frac{6\pi\eta a}{1 + A'(\ell/a)} v$$

$$F = 6\pi\eta v a\left[1 + (3/\sqrt{2})\phi^{1/2}\right]$$

$$F_N = 6\pi N \frac{\ell^2}{\kappa_0} \frac{a}{1 + A'(\ell/a)}\left(1 + \frac{3}{\sqrt{2}}\sqrt{c}\right) q = A(\Delta T)$$

$$\kappa_{eff} = \kappa_0 \frac{1}{\frac{1}{f(\phi)} + \frac{9}{2}\phi \frac{(\ell/a)^2}{1 + A'(\ell/a)}(1 + \frac{3}{\sqrt{2}}\sqrt{\phi})}$$

Porosity (%)	radius (nm)	κ_{eff} $Wm^{-1}K^{-1}$	Eq (6)	Standard
40	1,5	1.2	2.1	32
40	100	31.2	29.6	32
50	10	3.9	5.9	18.5
60	10	2,5	4.0	9.5

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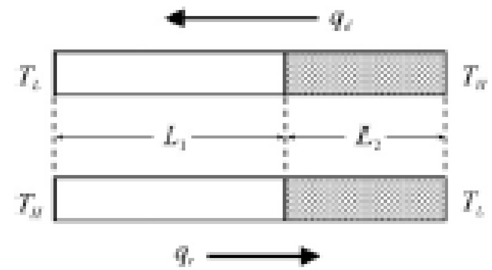
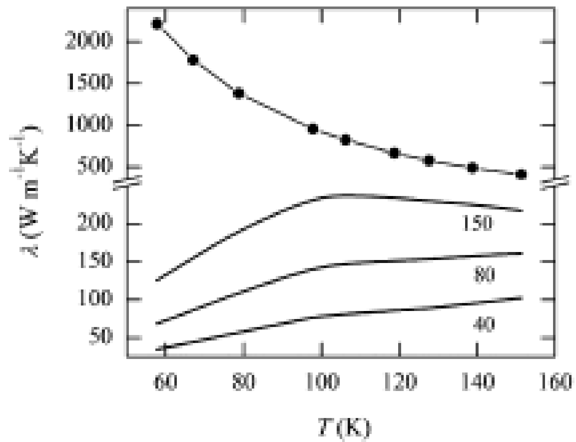
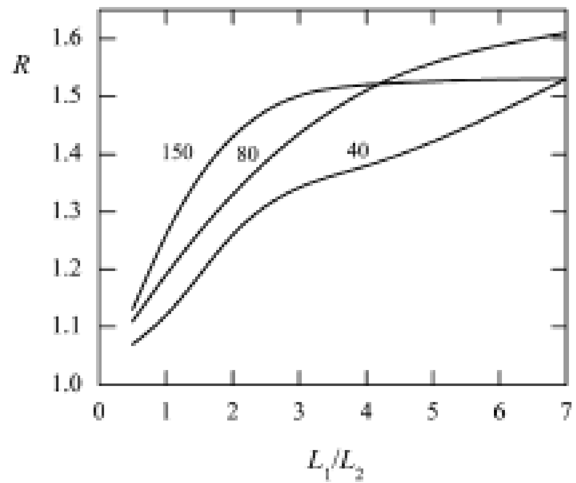
Pore-size dependence of the thermal conductivity of porous silicon: A phonon hydrodynamic approach

F. X. Alvarez,[1,a)] D. Jou,[1,2,b)] and A. Sellitto[3,c)]

PHONONICS:
THERMAL DIODES, THERMAL TRANSISTORS
THERMAL RECTIFICATION IN BULK-POROUS SI







Physics Letters A 376 (2012) 1641–1644

Theoretical analysis of thermal rectification in a bulk Si/nanoporous Si device

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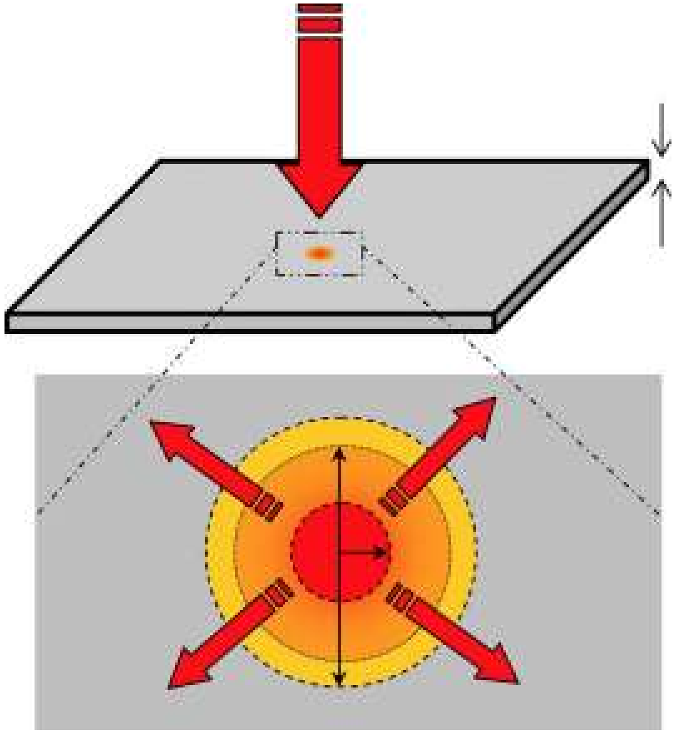
RADIAL HEAT TRANSPORT IN PLANE LAYERS: NANOREFRIGERATION



$$\tau_R \dot{\mathbf{q}} + \mathbf{q} = -\lambda_0 \nabla T + \ell^2 (\nabla^2 \mathbf{q} + 2\nabla\nabla \cdot \mathbf{q}),$$

$$q(r) = \frac{\Gamma}{r},$$

$$\lambda_0 \frac{\mathrm{d}T}{\mathrm{d}r} = -\frac{\Gamma}{r} + \ell^2 \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left[r \frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{\Gamma}{r}\right)\right] = \Gamma\left(\frac{\ell^2}{r^3} - \frac{1}{r}\right).$$

TEMPERATURE PROFILE AND SECOND LAW

$$\lambda_0 \frac{\mathrm{d}T}{\mathrm{d}r} = -\frac{\Gamma}{r} + \ell^2 \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left[r\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{\Gamma}{r}\right)\right] = \Gamma\left(\frac{\ell^2}{r^3} - \frac{1}{r}\right).$$

$$\Delta T(r) = \frac{\Gamma}{2\lambda_{\mathrm{eff}}}\frac{\ell^2}{r_0^2}\left(1 - \frac{r_0^2}{r^2}\right),$$

$$\sigma_{\mathrm{le}} = \mathbf{q} \cdot \nabla T^{-1},$$

$$\sigma_{\mathrm{eit}} = \mathbf{q} \cdot \nabla T^{-1} + \frac{\ell^2}{\lambda_0 T^2}\mathbf{q} \cdot \nabla^2 \mathbf{q} + \frac{\ell^2}{\lambda_0 T^2}\nabla \mathbf{q} : \nabla \mathbf{q} \geq 0,$$

Non-local effects in radial heat transport in silicon thin layers and graphene sheets

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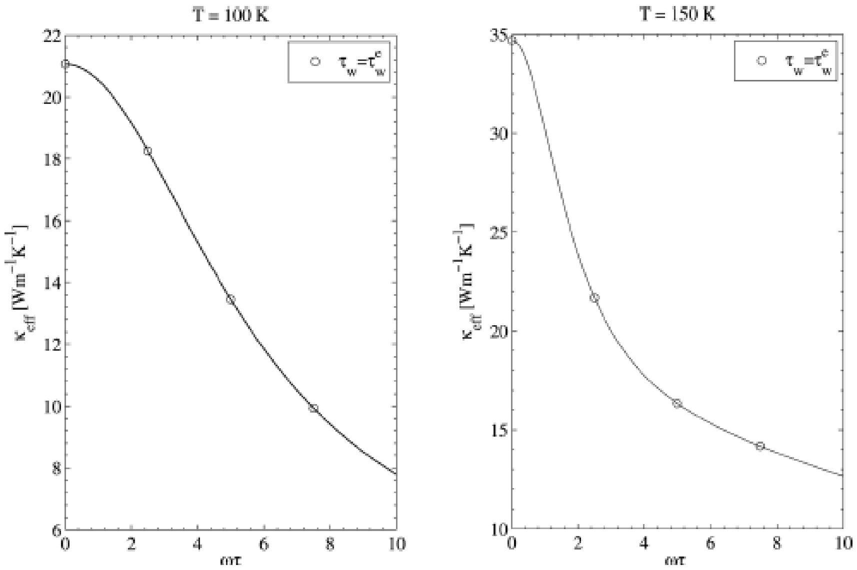
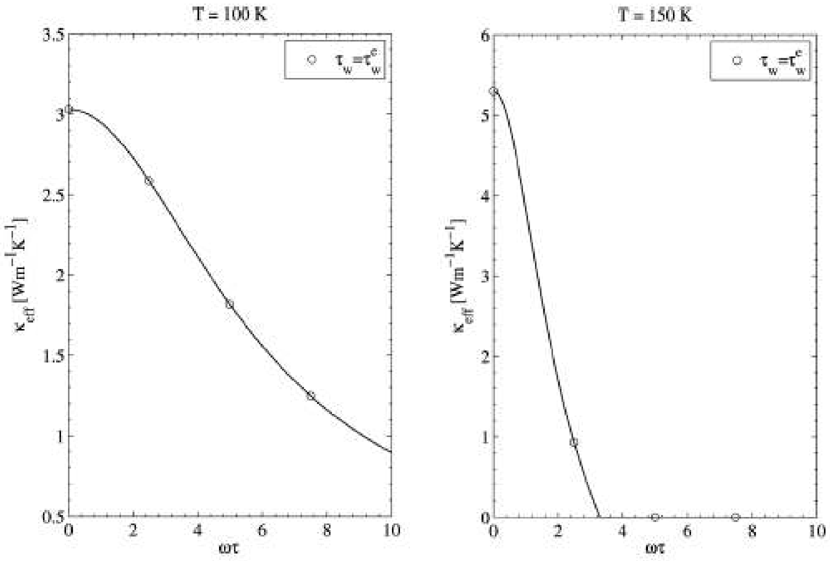
FREQUENCY-DEPENDENT THERMAL CONDUCTIVITY

$$\tau\dot{\mathbf{q}}+\mathbf{q}=-\kappa_0\nabla T,\qquad \kappa(\omega)=\frac{\kappa_0}{1+\omega^2\tau^2}.\qquad \tau\dot{\mathbf{q}}+\mathbf{q}=-\kappa_0\nabla T+\ell^2\left(\nabla^2\mathbf{q}+2\nabla\nabla\cdot\mathbf{q}\right),$$





JOURNAL OF APPLIED PHYSICS 109, 064317 (2011)

Phonon-wall interactions and frequency-dependent thermal conductivity in nanowires

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CONTINUED-FRACTION EXPANSIONS OF TRANSPORT COEFFICIENTS

$$\lambda(k) = \cfrac{\lambda_0(T)}{1 + \cfrac{k^2\ell_1^2}{1 + \cfrac{k^2\ell_2^2}{1 + \cfrac{k^2\ell_3^2}{1 + \dots}}}}$$

$$\lambda(L) = \frac{\lambda_0 L^2}{2\pi^2 l^2}\left[\sqrt{1 + 4\left(\frac{\pi l}{L}\right)^2} - 1\right].$$

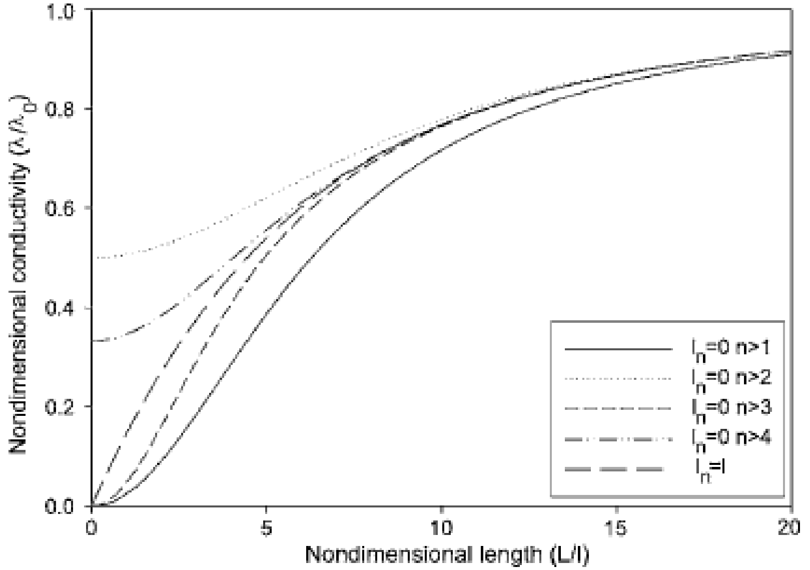

FIG. 5. Comparison plot between different expressions obtained from Eq. (1) depending of the number of nonvanishing l_n values. The difference between even and odd order approximations and the asymptotic behavior is seen.

ASYMPTOTIC EXPRESSION OF THERMAL CONDUCTIVITY

$$\lambda(L) = \frac{\lambda_0 L^2}{2\pi^2 l^2}\left[\sqrt{1+4\left(\frac{\pi l}{L}\right)^2} - 1\right].$$

$$L^{-2} = L_x^{-2} + L_y^{-2} + L_z^{-2}.$$

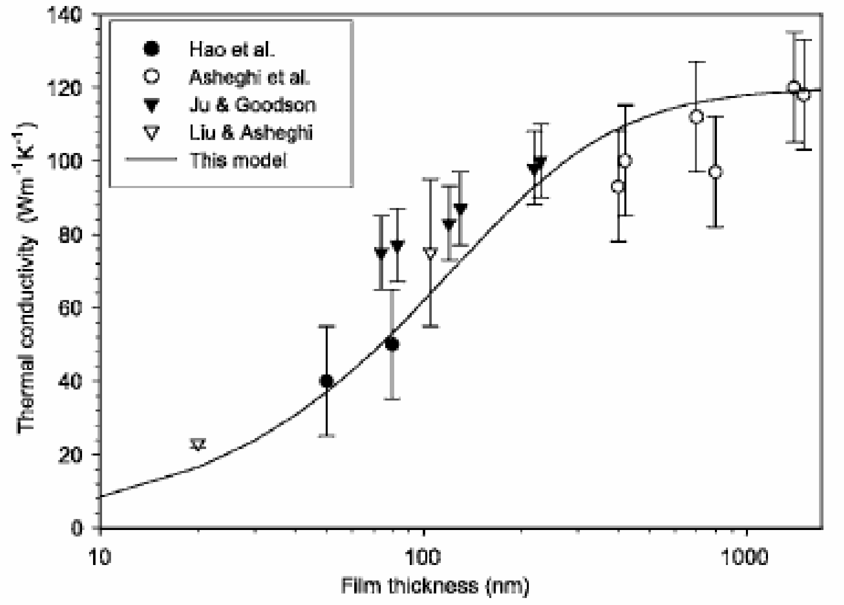

FIG. 1. Effective-thermal conductivity (λ) in W/(m K) given by Eq. (8) in terms of the width of the layer (L) in nm. The values used in the graph are 120 W/(cm K) for the asymptotic conductivity λ_0 and 40 nm for l. The points correspond to the experimental data in layers with different thicknesses (see Refs. 16 and 17).

CONCLUSIONS

- Non-local effects may be relevant in heat transport in nanosystems
- Generalized transport equations require generalized entropy and entropy flux
- Non-local effects are not always equivalent to Fourier's law with an effective thermal conductivity
- Several possibles descriptions: a) Effective relaxation time, b) Non-local effects + heat slip along the walls; c) Asymptotic many-fluxes expressions

SOME BOOKS

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