seminar on thermal transport

Professor Li Shi
University Texas Austin
"Thermal Transport in Nanostructured and Complex Materials"

Friday October 21, 2011 3:30pm PHYS 203

This seminar will review several intriguing quantum and classical size effects on thermal properties of nanostructured and complex materials. Topics to be discussed include the Casimir limit of lattice thermal conductivity of nanowires, the interplay between phonon-interface scattering and crystal complexity in III-V and silicide nanostructures, size-dependent thermal conductivity of carbon nanotubes and graphene, the effects of interface interaction on phonon transport in and across nanotubes and graphene, and local temperatures of different phonon populations in electrically biased carbon electronic devices. A current effort of developing bulk silicide thermoelectric waste heat recovery devices will be briefly introduced as an example of the engineering relevance of these fundamental studies in thermal physics.

no class on Monday, Oct. 24, 2011

Devices for high performance computing beyond 14 nm node - is there anything other than Si?

Please join us as Purdue welcomes Wilfried Haensch
Senior Manager
Devices & Materials for Advanced Logic and Communication, IBM

for the **Philip F. Bagwell Lecture**
Celebrating the memory of Philip Bagwell, former associate professor in Electrical and Computer Engineering.

PURDUE UNIVERSITY
SCHOOL OF ELECTRICAL AND COMPUTER ENGINEERING

Monday, October 24, 2011
2:00 p.m.
Burton Morgan Center
Room 121

The success of the microelectronic industry over the last several decades is related to the scalability of the MOSFET transistor. Since its conception in the late 1920, its first realization in the late 1950's, it took another 20 years for this device to become mainstream technology. After a short review on the history related to the MOSFET and device scaling I will talk about possible extensions of Si device technology, which are under consideration for 14nm and beyond. I will close the talk with a discussion of carbon-nano-tube based MOSFET devices.

no class on Monday, Oct. 24, 2011

Instead, view

ECE 656 F2009: Lecture 23: Phonon Scattering I

http://nanohub.org/resources/7780

ECE-656: Fall 2011

Lecture 23:

Ionized Impurity Scattering: II

Mark Lundstrom
Purdue University
West Lafayette, IN USA

10/19/11

Brooks-Herring II scattering

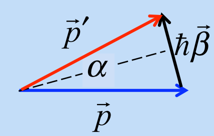
$$S(\vec{p},\vec{p}')=\frac{2\pi}{\hbar}\left|H_{p',p}\right|^2\delta(E'-E) \qquad H_{p,p'}=\frac{1}{\Omega}\tilde{U}_S(\beta)$$

$$U_S(r)=\frac{q^2}{4\pi\kappa_S\varepsilon_0 r}e^{-r/L_D}$$

$$\tilde{U}_S(\beta)=\frac{q^2}{\kappa_S\varepsilon_0}\frac{1}{\left(\beta^2+1/L_D^2\right)}$$

$$S(\vec{p},\vec{p}')=\frac{2\pi q^4 N_I}{\hbar\kappa_S^2\varepsilon_0^2\Omega}\frac{\delta(E'-E)}{\left(\beta^2+1/L_D^2\right)^2}$$

$$\vec{p}'=\vec{p}+\hbar\vec{\beta}$$



$$\frac{\hbar\beta}{2}=p\sin\alpha/2$$

examine result

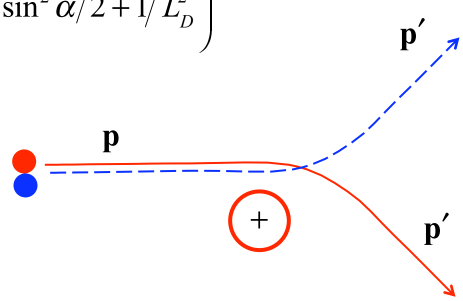
$$S(\vec{p},\vec{p}')=\frac{2\pi q^4 N_I}{\hbar\kappa_S^2\varepsilon_0^2\Omega}\frac{\delta(E'-E)}{\left(\frac{8m^*E}{\hbar^2}\sin^2\alpha/2+1/L_D^2\right)^2}$$

1) $S(\vec{p},\vec{p}')\sim N_I$

2) $S(\vec{p},\vec{p}')\sim q^4$

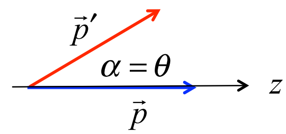
3) $S(\vec{p},\vec{p}')\sim 1/E^2$

4) favors small angle scattering



momentum relaxation time

$$\frac{1}{\tau_m} = \sum_{\vec{p}'} S(\vec{p}, \vec{p}')(1 - \cos\alpha)$$



$$\tau_m(E) = \frac{16\sqrt{2m^*}\pi\kappa_S^2\varepsilon_0^2}{N_I q^4}\left[\ln(1+\gamma^2) - \frac{\gamma^2}{1+\gamma^2}\right]E^{3/2}$$

$$\gamma^2 = 8m^* E L_D^2 / \hbar^2$$

See Lundstrom, FCT, pp. 69-70

$$\tau_m(E) \sim E^{3/2}$$

$$\tau_m(E) \approx \tau_0 \left(E/k_B T_L\right)^{3/2} \qquad \tau_0 \sim T_L^{3/2} \qquad s = 3/2$$

to be continued in next lecture

1) Review
2) **Conwell-Weisskopf approach**
3) II Mobility
4) Discussion
5) Summary / Questions

(Reference: Chapter 2, Lundstrom, FCT)

BH vs.CW

Brooks-Herring means “screened Coulomb scattering.”

Conwell-Weisskopf means “unscreened Coulomb scattering.”

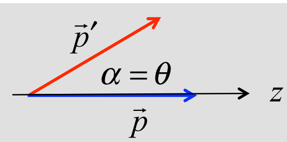
Conwell-Weiskopf approach

$$S(\vec{p},\vec{p}\,') = \frac{2\pi q^4 N_I}{\hbar \kappa_S^2 \epsilon_0^2 \Omega} \frac{\delta(E' - E)}{\left(\frac{8m^* E}{\hbar^2}\sin^2\alpha/2\right)^2}$$

unscreened Coulomb potential

$$S(\vec{p},\vec{p}\,') \to \infty \quad \text{as} \quad \alpha \to 0$$

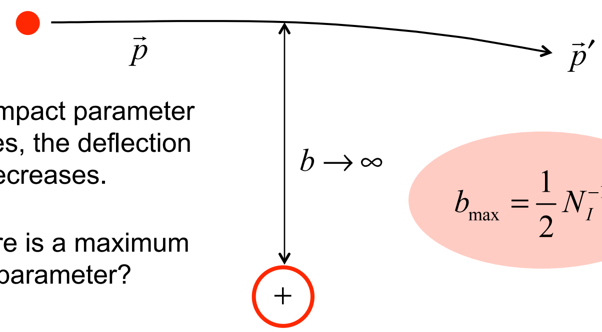
$$\frac{1}{\tau_m} = \sum_{\vec{p}\,'} S(\vec{p},\vec{p}\,')(1-\cos\alpha)$$



Can we specify a minimum angle, so that the integral does not blow up?

Conwell-Weiskopf approach

$$S(\vec{p},\vec{p}\,') = \frac{2\pi q^4 N_I}{\hbar \kappa_S^2 \varepsilon_0^2 \Omega} \frac{\delta(E' - E)}{\left(\frac{8m^* E}{\hbar^2}\sin^2 \alpha/2\right)^2}$$



As the impact parameter increases, the deflection angle decreases.

But there is a maximum impact parameter?

$$b_{\max} = \frac{1}{2} N_I^{-1/3}$$

Conwell-Weisskopf approach

$$\frac{1}{\tau_m} = \sum_{\vec{p}\,'} S(\vec{p},\vec{p}\,')(1-\cos\alpha)$$

$$\frac{1}{\tau_m} = \frac{\Omega}{(2\pi)^3} \int_0^{2\pi} d\phi \int_{\alpha_{\min}}^{\pi} S(\vec{p},\vec{p}\,')(1-\cos\alpha)\sin\alpha\, d\alpha\, p'^2 dp' =$$

$$b_{\max} = \frac{q^2}{8\pi\kappa_S \varepsilon_0 E(p)} \cot(\alpha_{\min}/2) \qquad \text{(Rutherford)}$$

Conwell-Weisskopf approach

$$\frac{1}{\tau_m} = \sum_{\vec{p}'} S(\vec{p}, \vec{p}')(1 - \cos\alpha)$$

$$\tau_m(E) = \frac{16\pi\sqrt{2m^*}\kappa_S^2\varepsilon_0^2}{N_I q^4}\left[\frac{1}{\ln\left(1+\gamma_{CW}^2\right)}\right]E^{3/2} \qquad \gamma_{CW}^2 = b_{\max}\Big/\left(q^2/8\pi\kappa_S\varepsilon_0 E\right)$$

$\tau_m(E) \sim E^{3/2}$ See Lundstrom, FCT, pp. 70-73

$$\tau_m(E) \approx \tau_0\left(E/k_B T_L\right)^{3/2} \qquad \tau_0 \sim T_L^{3/2} \qquad s = 3/2$$

Much like the Brooks-Herring result.

CW vs. BH

Compare b_{MAX} to L_D

Use BH if:

$$b_{\max} > L_D$$

$$b_{\max} = \frac{1}{2}N_I^{-1/3}$$

$$L_D = \sqrt{\frac{\kappa_S\varepsilon_0 k_B T}{q^2 n_0}}$$

B. K. Ridley, "Reconciliation of the Conwell-Weisskopf and Brooks-Herring formulae for charged-impurity scattering in semiconductors: Third-body interference," *J. Phys. C: Solid State Phys*. **10,** p. 1589 doi:10.1088/0022-3719/10/10/003, 1977.

outline

1) Review
2) Conwell-Weisskopf approach
3) **II Mobility**
4) Discussion
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(Reference: Chapter 2, Lundstrom, FCT)

Brooks-Herring

$$\tau_m(E) = \frac{16\sqrt{2m^*}\pi\kappa_S^2\varepsilon_0^2}{N_I q^4}\left[\ln\left(1+\gamma^2\right) - \frac{\gamma^2}{1+\gamma^2}\right]E^{3/2}$$

$$\gamma^2 = 8m^* E L_D^2 / \hbar^2$$

(Lecture 15)

$$\mu_n = q\frac{\langle\langle\tau_m(E)\rangle\rangle}{m^*} \qquad \tau_m(E) = \tau_0\left(E/k_BT\right)^s$$

$$\langle\langle\tau_m(E)\rangle\rangle = \frac{\langle E\tau_m(E)\rangle}{\langle E\rangle} \qquad \langle X\rangle \equiv \frac{\sum_k X(E)f_0(E)}{\sum_k f_0(E)} \qquad \langle\langle\tau_m\rangle\rangle = \tau_0\frac{\Gamma(s+5/2)}{\Gamma(5/2)}$$

Brooks-Herring (ii)

$$\tau_m(E) = \frac{16\sqrt{2m^*}\pi\kappa_S^2\varepsilon_0^2}{N_I q^4}\left[\ln\left(1+\gamma^2\right) - \frac{\gamma^2}{1+\gamma^2}\right]E^{3/2}$$

$$\gamma^2 = 8m^* E L_D^2/\hbar^2 \qquad \gamma_{BH}^2 = 8m^* \hat{E} L_D^2/\hbar^2 \qquad \tau_m\left(E\right) = \tau_0\left(\hat{E}\right)\left(E/k_B T\right)^s$$

(Lecture 15)

maximum of integrand occurs at $\hat{E} = \left(s + 3/2\right)k_B T_L$

$$\mu_n = q\frac{\langle\langle\tau_m(E)\rangle\rangle}{m^*}$$

$$\tau_m\left(E\right) = \tau_0\left(E/k_B T\right)^s$$

$$\langle\langle\tau_m(E)\rangle\rangle = \frac{\langle E\tau_m\left(E\right)\rangle}{\langle E\rangle} \qquad \langle X\rangle \equiv \frac{\sum_k X\left(E\right)f_0\left(E\right)}{\sum_k f_0\left(E\right)} \qquad \langle\langle\tau_m\rangle\rangle = \tau_0\frac{\Gamma\left(s+5/2\right)}{\Gamma\left(5/2\right)}$$

Brooks-Herring (ii)

$$\tau_m(E) = \frac{16\sqrt{2m^*}\pi\kappa_S^2\varepsilon_0^2\left(k_B T_L\right)^{3/2}}{N_I q^4}\left[\ln\left(1+\gamma_{BH}\right) - \frac{\gamma_{BH}}{1+\gamma_{BH}}\right]\left(\frac{E}{k_B T_L}\right)^{3/2}$$

$$\gamma_{BH}^2 = 8m^* \hat{E} L_D^2/\hbar^2 \qquad \tau_m\left(E\right) = \tau_0\left(\hat{E}\right)\left(E/k_B T\right)^s \qquad \hat{E} = \left(s+3/2\right)k_B T_L$$

$$\mu_n = q\frac{\langle\langle\tau_m(E)\rangle\rangle}{m^*}$$

$$\langle\langle\tau_m\rangle\rangle = \tau_0\left(\hat{E}\right)\frac{\Gamma\left(s+5/2\right)}{\Gamma\left(5/2\right)}$$

$$\mu_{BH} = \frac{128\sqrt{2\pi}\kappa_S^2\varepsilon_0^2\left(k_B T_L\right)^{3/2}}{q^3\sqrt{m^*}N_I\left[\ln\left(1+\gamma_{BH}^2\right) - \gamma_{BH}^2/\left(1+\gamma_{BH}^2\right)\right]}$$

(Lundstrom, FCT, Sec. 4.8.1)

Conwell-Weiskopf

$$\tau_m(E) = \frac{16\pi\sqrt{2m^*}\kappa_S^2\varepsilon_0^2\left(k_BT_L\right)^{3/2}}{N_I q^4}\left[\frac{1}{\ln\left(1+\gamma_{CW}^2\right)}\right]\left(\frac{E}{k_BT_L}\right)^{3/2}$$

$$\gamma_{CW}^2 = b_{\max}\Big/\left(q^2/8\pi\kappa_S\varepsilon_0\hat{E}\right) \qquad b_{\max} = \frac{1}{2}N_I^{-1/3} \qquad \tau_m\left(E\right) = \tau_0\left(\hat{E}\right)\left(E/k_BT\right)^s$$

$$\mu_n = q\frac{\langle\langle\tau_m(E)\rangle\rangle}{m^*}$$

$$\langle\langle\tau_m\rangle\rangle = \tau_0\left(\hat{E}\right)\frac{\Gamma\left(s+5/2\right)}{\Gamma\left(5/2\right)}$$

$$\mu_{BH} = \frac{128\sqrt{2\pi}\kappa_S^2\varepsilon_0^2\left(k_BT_L\right)^{3/2}}{q^3\sqrt{m^*}N_I\left[\ln\left(1+\gamma_{CW}^2\right)\right]}$$

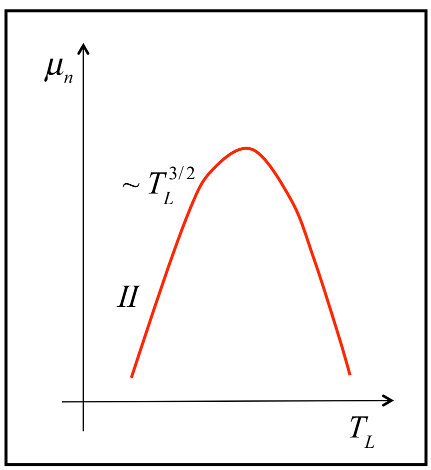
(Lundstrom, FCT, prob. 4.17)

mobility

$$\mu_n = \frac{q\langle\langle\tau_m\rangle\rangle}{m^*} = \frac{q\tau_0}{m^*}\frac{\Gamma\left(s+5/2\right)}{\Gamma\left(5/2\right)}$$

$\tau_0 \propto T_L^{3/2}$ $\qquad s = 3/2$

$\mu_n \propto T_L^{3/2}$



$T^{3/2}$ temperature dependence is the "signature" of charged impurity scattering.

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Hall factor for II scattering

$$r_H \equiv \langle\langle \tau_m^2 \rangle\rangle / \langle\langle \tau_m \rangle\rangle^2 \qquad s = 3/2$$

$$\tau_m = \tau_0 \left(E/k_B T_L\right)^s \qquad \tau_m^2 = \tau_0^2 \left(E/k_B T_L\right)^{2s}$$

$$\langle\langle \tau_m \rangle\rangle = \tau_0 \frac{\Gamma(s+5/2)}{\Gamma(5/2)}$$

$$\langle\langle \tau_m^2 \rangle\rangle = \tau_0^2 \frac{\Gamma(2s+5/2)}{\Gamma(5/2)}$$

$$r_H = \frac{\Gamma(2s+5/2)\Gamma(5/2)}{\left[\Gamma(s+5/2)\right]^2} = 1.93$$

$$\langle\langle \tau_m(E) \rangle\rangle = \frac{\langle E\tau_m(E) \rangle}{\langle E \rangle}$$

$$\langle\langle \tau_m \rangle\rangle = \tau_0 \frac{\Gamma(s+5/2)}{\Gamma(5/2)}$$

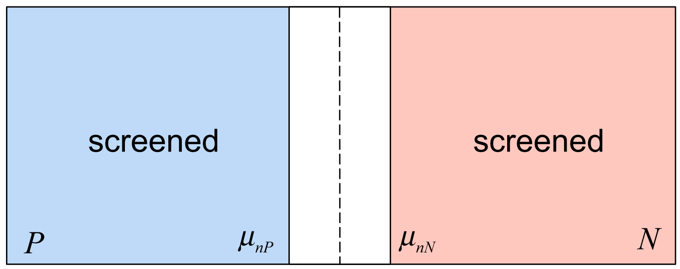
$\Gamma(n) = (n-1)!$ (*n* integer)

$\Gamma(1/2) = \sqrt{\pi}$

$\Gamma(p+1) = p\Gamma(p)$

PN junction

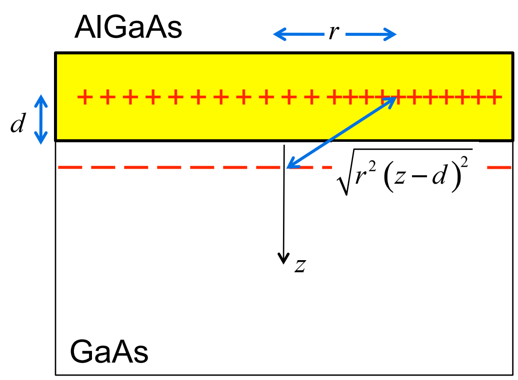
$$U_S(r) = +\frac{q^2}{4\pi\kappa_S\varepsilon_0 r}e^{-r/L_D} \qquad U_S(r) = -\frac{q^2}{4\pi\kappa_S\varepsilon_0 r}e^{-r/L_D}$$



unscreened

$$U_S(r) = +\frac{q^2}{4\pi\kappa_S\varepsilon_0 r} \qquad U_S(r) = -\frac{q^2}{4\pi\kappa_S\varepsilon_0 r}$$

screening 2D modulation-doped layers



The heterojunction interface can be atomically smooth and at low temperatures, phonon scattering is absent, **so scattering by remote impurities dominates**. Extraordinarily high mobilities (e.g. > 10^6 cm^2/V-s) can be achieved at about T_L = 1K.

modulation-doped structures

For a discussion of modulation doping, screening in 2D, and remote impurity scattering in 2D, see:

J.H. Davies, *The Physics of Low-Dimensional Semiconductors*, Chapter 8, Cambridge Univ. Press, 1998.

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(Reference: Chapter 2, Lundstrom, FCT)

summary

1) The two classic treatments of II scattering are Brooks-Herring and Conwell-Weiskopf

2) II scattering is actually difficult to treat properly because:

   FGR does not account for the difference in sign of the scattering potential

   "multiple scattering" occurs at heavy doping.

summary

3) For a bulk semiconductor, II scattering can be described (approximately) in a power law form with a characteristic exponent of 3/2.

4) A mobility that increases as $T_L^{3/2}$ is the "signature" of II scattering.

5) The low temperature mobility is often used as a measure of the total ionized impurity concentration in a sample.

questions

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