Lecture10:
Mobility calculation

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On this Wednesday

- Invited talk in the Korean Physics Society meeting in Gwangju
  - We need to change the lecture time.
  - I can come back Wednesday evening.
  - *Are you available?*

Homework#4

- Due: October 19th

- Repeat Homework#3 with realistic band structures.
  - a) Ellipsoidal model without non-parabolicity
    - $m_l = 0.914$
    - $m_t = 0.196$
  - b) Consider the non-parabolicity ($\alpha = 0.5$ eV^{-1})
    - How can we consider the non-parabolicity?
- Extension to 2D cross section.
  - 20 nm by 10 nm
- Calculate the bulk hole band structure.
  - For a while, neglect the strain terms.

Note that

- Change of lecture coverage
  - Mobility calculator
  - Multi-subband BTE solver
  - Drift-diffusion simulator and its application

- Omitted topics
  - NEGF
  - SHE
  - FDTD

Band structure of Si (1)

- Conduction band
  - Ellipsoidal model

$$E(\mathbf{k}) = \frac{\hbar^2 k_z^2}{2m_l} + \frac{\hbar^2}{2m_t}\left(k_x^2 + k_y^2\right)$$

  - Non-parabolicity

$$E^{NP}(\mathbf{k})\left(1 + \alpha E^{NP}(\mathbf{k})\right) = E(\mathbf{k})$$

Band structure of Si (2)

- Valence band
  - Six-band k.p model (Taken from S-Band manual)

$$
H_{LK} = -\begin{array}{c|cccccc|c}
 & \left|\frac{3}{2},\frac{3}{2}\right\rangle & \left|\frac{3}{2},\frac{1}{2}\right\rangle & \left|\frac{3}{2},-\frac{1}{2}\right\rangle & \left|\frac{3}{2},-\frac{3}{2}\right\rangle & \left|\frac{1}{2},\frac{1}{2}\right\rangle & \left|\frac{1}{2},-\frac{1}{2}\right\rangle & \\
\hline
 & P+Q & -S & R & 0 & -\frac{S}{\sqrt{2}} & \sqrt{2}R & \left|\frac{3}{2},\frac{3}{2}\right\rangle \\
 & & P-Q & 0 & R & -\sqrt{2}Q & \sqrt{\frac{3}{2}}S & \left|\frac{3}{2},\frac{1}{2}\right\rangle \\
 & & & P-Q & S & \sqrt{\frac{3}{2}}S^{*} & \sqrt{2}Q & \left|\frac{3}{2},-\frac{1}{2}\right\rangle \\
 & & & & P+Q & -\sqrt{2}R^{*} & -\frac{S^{*}}{\sqrt{2}} & \left|\frac{3}{2},-\frac{3}{2}\right\rangle \\
 & & & & & P+\Delta & 0 & \left|\frac{1}{2},\frac{1}{2}\right\rangle \\
 & & & & & & P+\Delta & \left|\frac{1}{2},-\frac{1}{2}\right\rangle
\end{array}
$$

Complex conjugate

Band structure of Si (3)

- Valence band
  - Definitions
    - $P = P_k + P_\varepsilon \qquad Q = Q_k + Q_\varepsilon \qquad R = R_k + R_\varepsilon \qquad S = S_k + S_\varepsilon$

Luttinger–Kohn:

$$P_k = \frac{\hbar^2}{2m_0}\gamma_1(k_x^2 + k_y^2 + k_z^2)$$

$$Q_k = \frac{\hbar^2}{2m_0}\gamma_2(k_x^2 + k_y^2 - 2k_z^2)$$

$$R_k = \frac{\hbar^2}{2m_0}\sqrt{3}[-\gamma_2(k_x^2 - k_y^2) + 2i\gamma_3 k_x k_y]$$

$$S_k = \frac{\hbar^2}{2m_0}2\sqrt{3}\gamma_3(k_x - ik_y)k_z$$

Bir–Pikus:

$$P_\varepsilon = -a(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$

$$Q_\varepsilon = -\frac{b}{2}(\varepsilon_{xx} + \varepsilon_{yy} - 2\varepsilon_{zz})$$

$$R_\varepsilon = \frac{\sqrt{3}}{2}b(\varepsilon_{xx} - \varepsilon_{yy}) - id\varepsilon_{xy}$$

$$S_\varepsilon = -d(\varepsilon_{zx} - i\varepsilon_{yz})$$

- $\gamma_1, \gamma_2, \gamma_3$ are the Luttinger parameters.
- a, b, d are the Bir–Pikus deformation potentials.
- Δ is the spin-orbit split-off energy.

Band structure of Si (4)

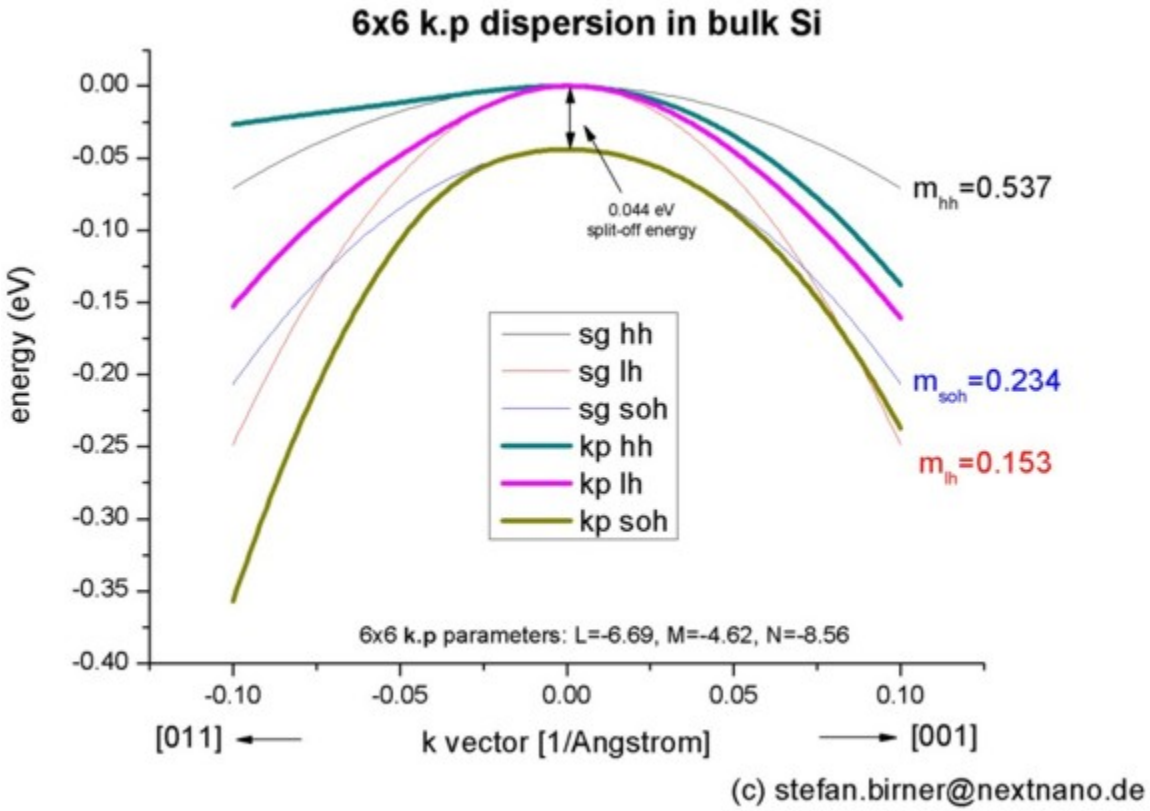
- Valence band
  - Parameters

Symbol	Parameter name	Si default value	Ge default value	Unit
γ_1	gamma1	4.306	10.536	1
γ_2	gamma2	0.345	3.107	1
γ_3	gamma3	1.44	4.397	1
Δ_{so}	Delta	0.0434	0.297	eV

Symbol	Parameter name	Si default value	Ge default value	Unit
a	a_v	2.46	1.25	eV
b	b	–2.316	–2.067	eV
d	d	–5.514	–3.836	eV

Band structure of Si (5)

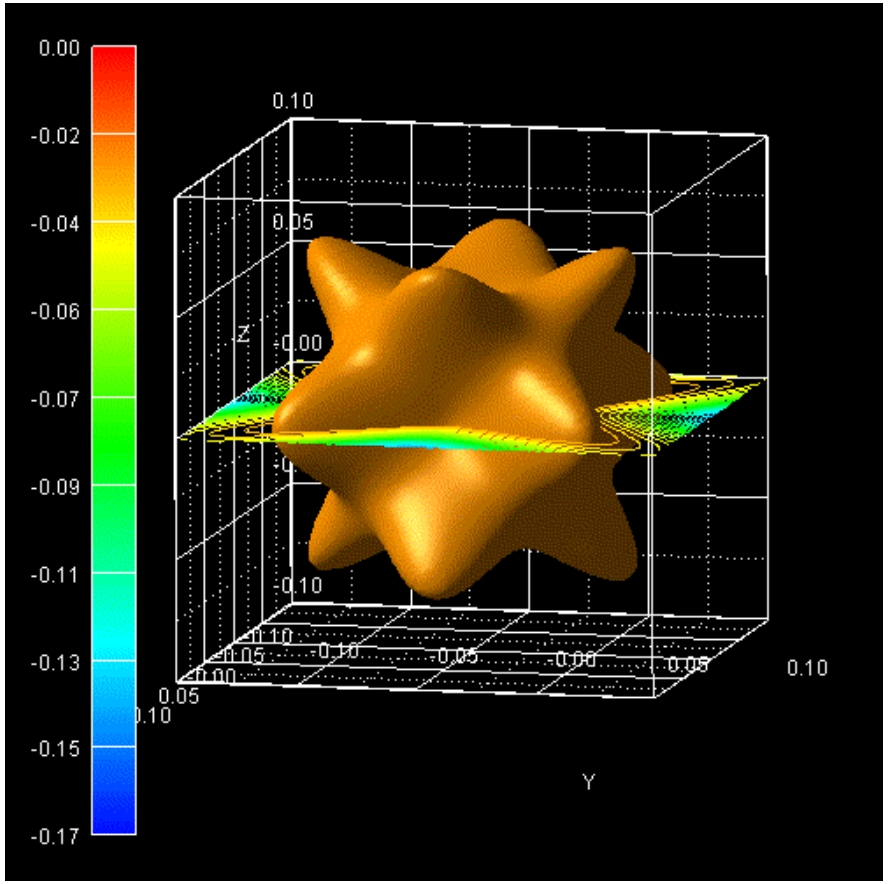
- Valence band
  - Results (taken from www.nextnano.com)

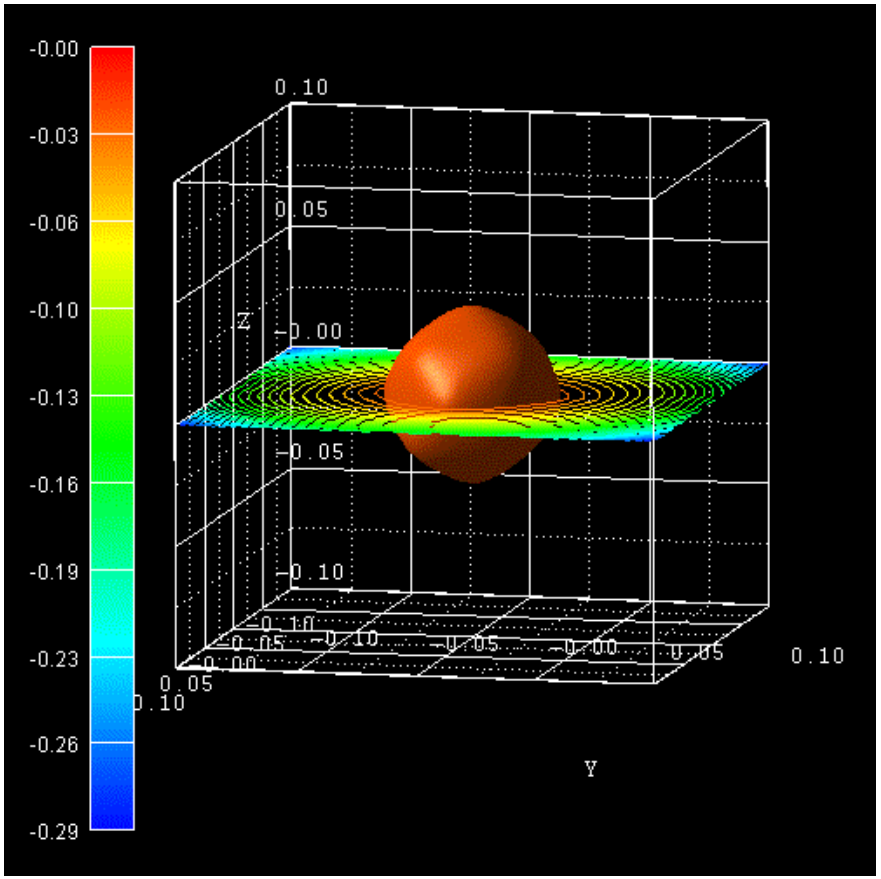


It is your Homework#4.

Band structure of Si (6)

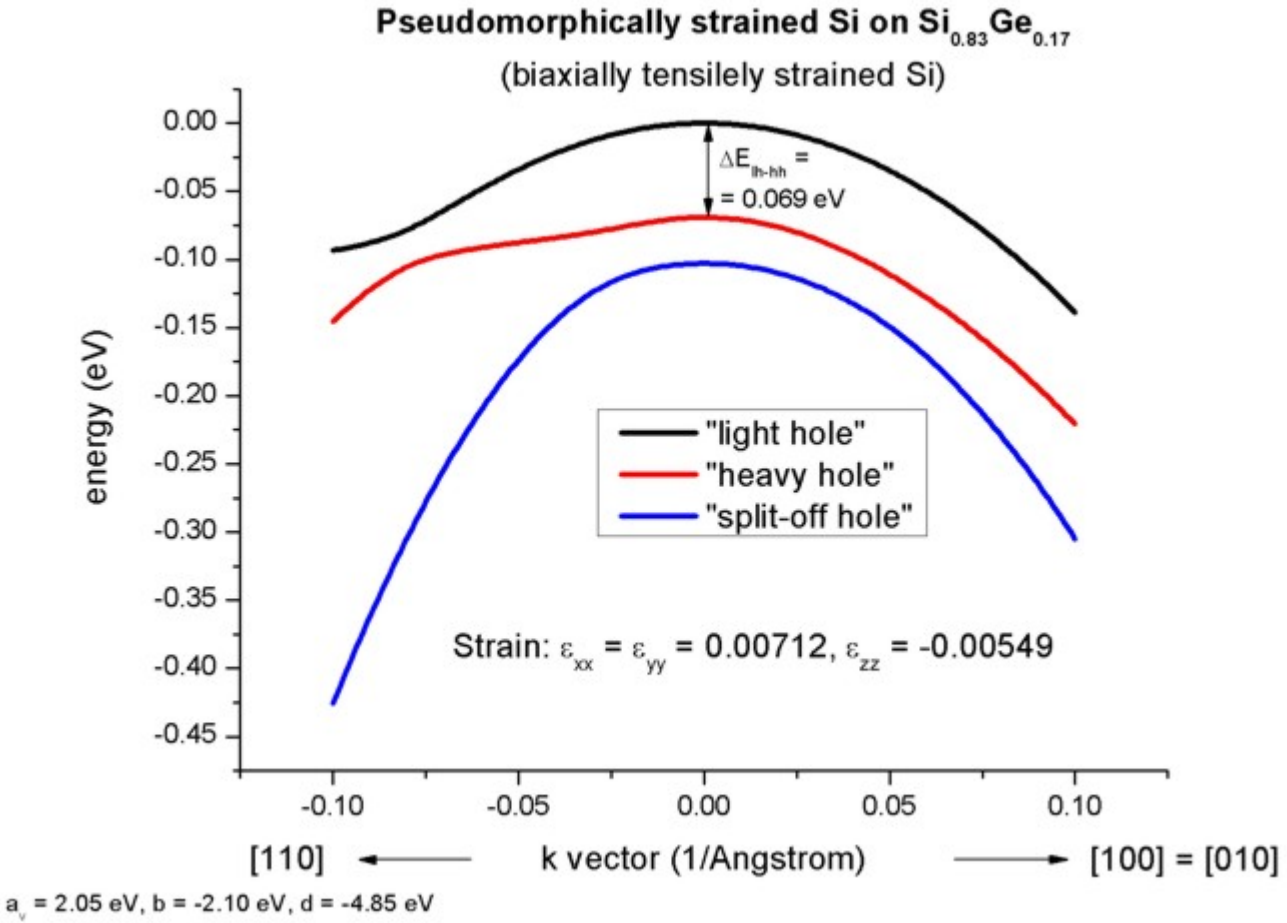
- Valence band
  - Results (taken from www.nextnano.com)





Band structure of Si (7)

- Valence band
  - Results (taken from www.nextnano.com)



Mobility calculation

- Up to now, we have considered the subband structure.
  - As much as the transport is concerned, the mobility is an important quantity.
  - We calculate the mobility in the following way (Kubo-Greenwood):

$$\mu_{ij}^{\nu} = \frac{e}{\hbar^2 k_B T} \frac{1}{N_\nu} \frac{g_\nu}{(2\pi)^d} \int d\boldsymbol{k}\, \tau_i^\nu \frac{\partial E_\nu}{\partial k_i} \frac{\partial E_\nu}{\partial k_j} f_0(E_\nu)[1 - f_0(E_\nu)]$$

- g_ν is the degeneracy.
- N_ν is the subband inversion carrier density.
- τ_i^ν is the total momentum relaxation time for subband ν in direction (i).
- E_ν is the subband energy dispersion.
- f_0 is the equilibrium Fermi–Dirac distribution function.
- d is the dimension of $\boldsymbol{k}$-space.

Momentum relaxation time

- The key parameter is the momentum relaxation time.

$$\frac{1}{\tau_i^{\nu}(\boldsymbol{k})} = \sum_{\nu'} \int \frac{d\boldsymbol{k}'}{(2\pi)^2} S_{\nu\boldsymbol{k},\,\nu'\boldsymbol{k}'} \times \Phi_i(\nu\boldsymbol{k},\,\nu'\boldsymbol{k}')$$

$$= \frac{2\pi}{\hbar} \sum_{\upsilon'} \int \frac{d\boldsymbol{k}'}{(2\pi)^d} \left|M_{\nu\boldsymbol{k},\,\nu'\boldsymbol{k}'}\right|^2 \delta(E_{\nu'}(\boldsymbol{k}') - E_{\nu}(\boldsymbol{k}) \mp \hbar\omega) \times \Phi_i(\nu\boldsymbol{k},\,\nu'\boldsymbol{k}')$$

where $S_{\nu\boldsymbol{k},\,\nu'\boldsymbol{k}'}$ is the transition rate between the initial wavevector $\boldsymbol{k}$ in subband ν and the final wavevector $\boldsymbol{k}'$ in subband ν'. The matrix element for scattering between initial and final states is denoted by $M_{\nu\boldsymbol{k},\,\nu'\boldsymbol{k}'}$ and $E_{\nu}(\boldsymbol{k})$ is the subband dispersion.

What we can do in the class

- Phonon-limited mobility

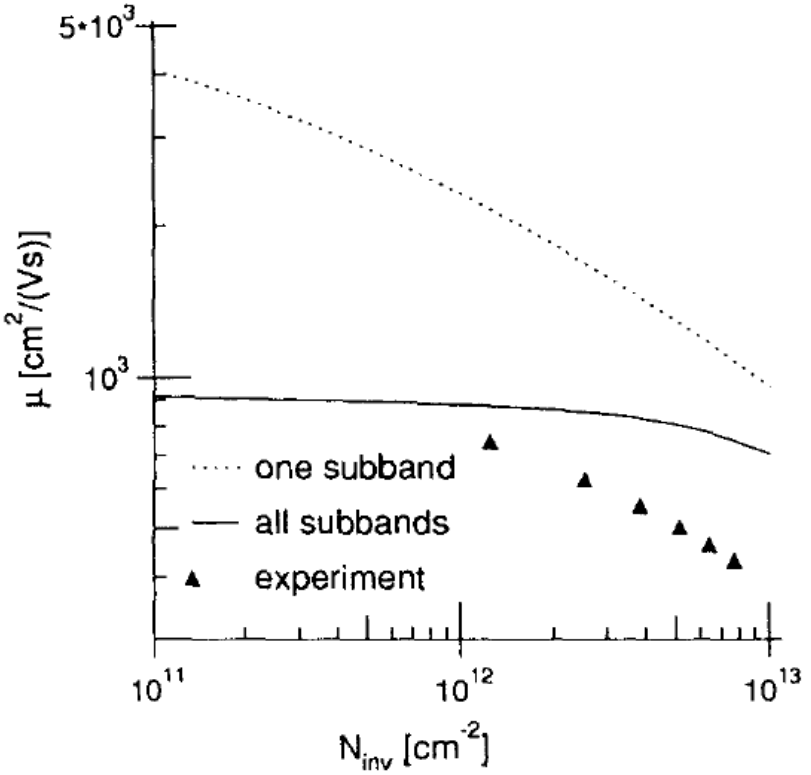


Fig. 4. The phonon limited mobility as a function of N_{inv}. The solid line is a result obtained with all relevant subbands, the dotted line is a result obtained with one subband and the triangles are experimental data[30]. ($N_A = 10^{14}/cm^3$ and 300 K.)

Taken from
Jungemann, SSE, vol. 36, pp. 1529-1540.
(It will be distributed in the class.)