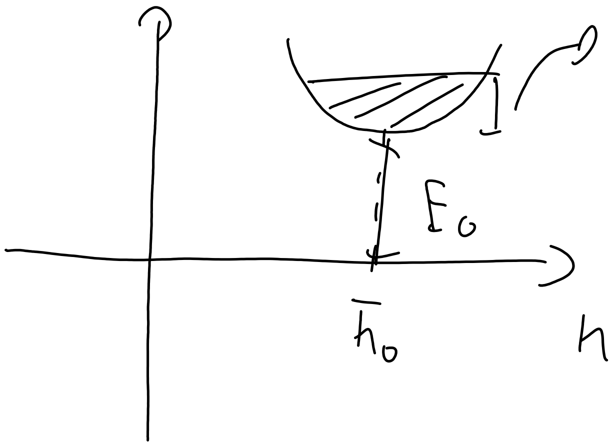
Effective mass

- Effective mass anisotropy → TENSOR
- Electron effective mass in multivalley semiconductors
- The conductivity effective mass
- The density of states effective mass
- Hole effective mass



$E(k) - E_0$

$$E(\vec{k}) = E_0(k_0) + \cancel{\frac{\partial E}{\partial k_x}(k_x - k_x}$$

$$+ \frac{1}{2}\frac{\partial^2 E}{\partial k_x^2}(k_x - k_{0x})^2 + \frac{1}{2}$$

$$\frac{\hbar^2 (k - k_0)^2}{2 m^*} \to \frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 E(k)}{\partial k_x^2}$$

$$E(k) - E_0 = + \hbar^2 (k_x - k_{0x})^2 + \hbar^2 (k_y - k_0$$

$\frac{\quad}{2m_x}(h_x - \quad x) \qquad \frac{\quad}{2m_y}(h_y$

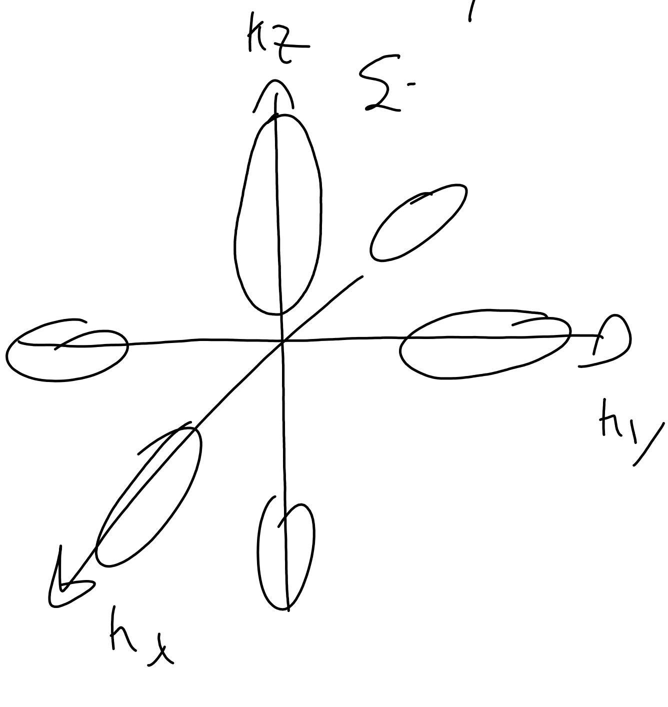
$$\boxed{1 = \frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2}}$$

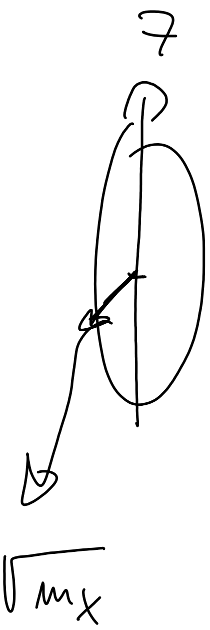
$a, b, c =$

ISO ENERGY $\qquad E(h) - E_0 = \bar{E}$

$$\boxed{1 = \frac{(h_x - h_{0x})^2}{\frac{2 m_x \bar{E}}{\hbar^2}} + \frac{(h_y - h_{0y})^2}{\frac{2 m_y \bar{E}}{\hbar^2}} +}$$

$$a = \frac{\sqrt{2 m_x \bar{E}}}{\hbar} \propto \sqrt{m_x}$$





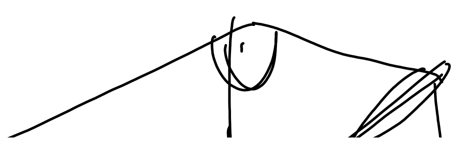
$$\bar{E} = \frac{\hbar^2 h_x^2}{2 m_t}$$

$m_t =$ Tra

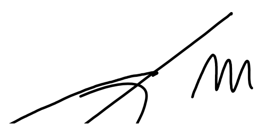
m

$m_l =$ lo

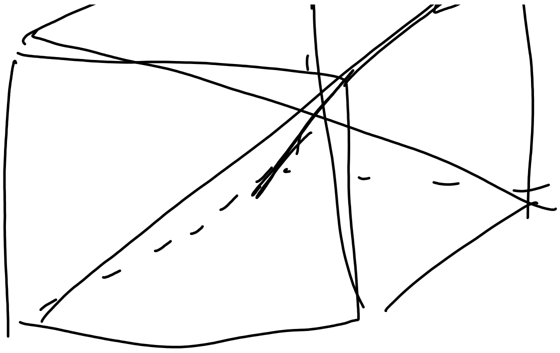
m

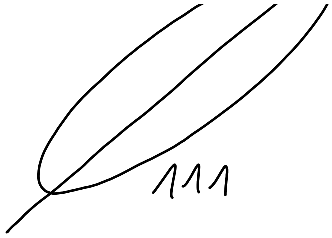


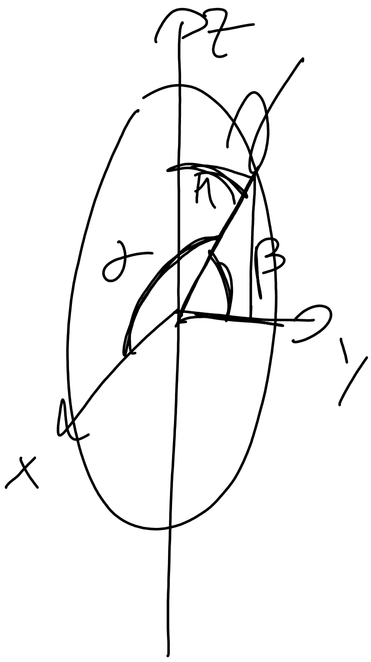
x 6



m







$$E = \frac{\hbar^2 k^2 \cdot \cos^2\alpha}{2m_l} + \frac{\hbar^2 k^2 \cos}{2m_l}$$

$$\frac{1}{m^*} = \frac{\cos^2\alpha}{m_l} + \frac{\cos^2\beta}{m_l} +$$

Effective mass

The bandstructure around a CB minimum can be expressed as :

$$E(\mathbf{k}) = \frac{\hbar^2 (k_x - k_{x0})^2}{2m_x} + \frac{\hbar^2 (k_y - k_{y0})^2}{2m_y} + \frac{\hbar^2 (k_z - k_{z0})^2}{2m_z}$$

Where m_x, m_y, m_z are the effective masses defined as:

$$\frac{1}{m_x} = \frac{1}{\hbar^2}\frac{\partial^2 E(\vec{k})}{\partial^2 k_x} \qquad \frac{1}{m_y} = \frac{1}{\hbar^2}\frac{\partial^2 E(\vec{k})}{\partial^2 k_y} \qquad \frac{1}{m_z} = \frac{1}{\hbar^2}\frac{\partial^2 E(\vec{k})}{\partial^2 k_z}$$

A high curvature radius in the bandstructure is associated with a “heavy” effective mass and a small curvature radius with a “light” effective mass

The effective mass along a given direction ***k*** with director cosines *n*, *l* and *m* is given by

$$\frac{1}{\hbar^2}\frac{\partial^2 E(\mathbf{k})}{\partial k^2} = \frac{1}{m_k} = \frac{n^2}{m_x} + \frac{l^2}{m_y} + \frac{m^2}{m_z}$$

$m = \cos\gamma$

$l = \cos\beta$

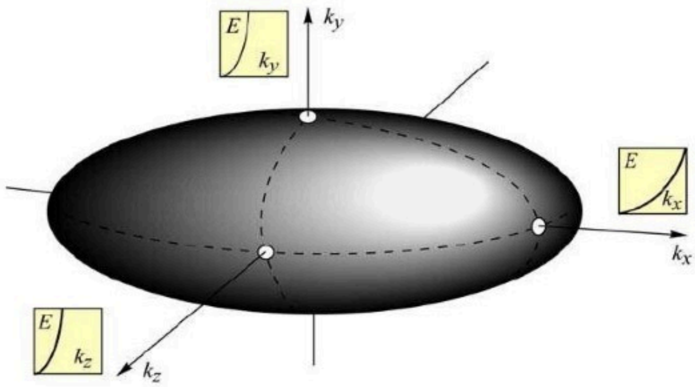
Si and Ge conduction band

Che CB of Si and Ge are characterized by two different effective masses named the longitudinal and transverse effective mass m_l and m_t. Let's consider the CB minimum placed at *0.85 π/a* along the [001] direction in the reciprocal space of Si. The longitudinal mass is the one related to transport in the [001] direction, the transverse mass is associated to transport in any direction perpendicular to [001] .

$$E(\vec{k}) = E(\vec{k}_0) + \frac{\hbar^2}{2}\left(\frac{k_z^2 + k_y^2}{m_t} + \frac{k_x^2}{m_l}\right)$$

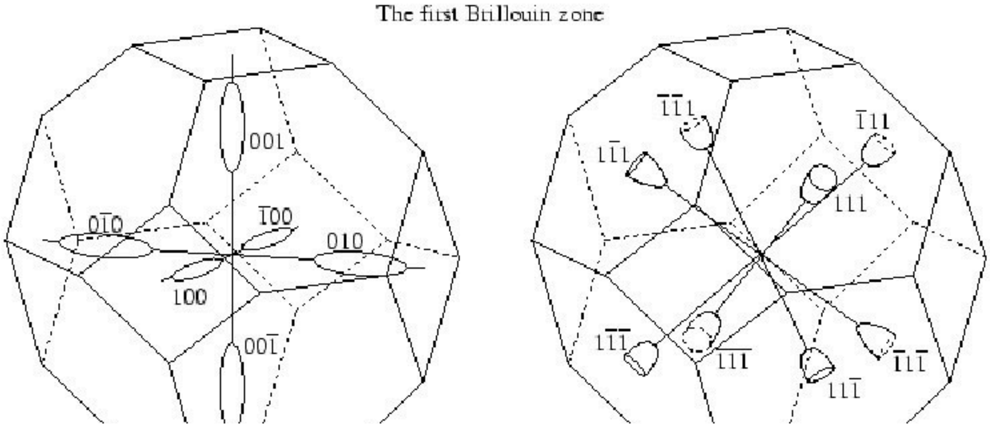
The isoenergetic surface will be an ellipsoid with semiaxes proportional to the square root of m_l and m_t .

In the case of Ge m_l will be along the [111] direction and m_t along any direction perpendicular to it.



Si and Ge conduction band

The first Brillouin zone



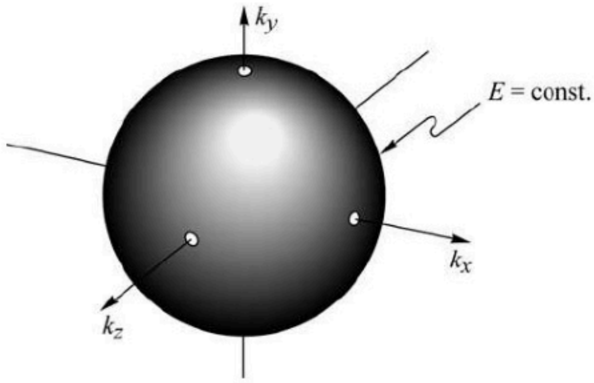
X valleys of Si　　　L valleys of Ge

$m_l = 0.98\, m_0$　　$m_t = 0.19\, m_0$　　$m_l = 1.64\, m_0$　　$m_t = 0.082\, m_0$

GaAs conduction band

The CB of GaAs features a single minimum at Γ. The isoenergetic surface is, in the parabolic approximation, a sphere with:

$$E(\vec{k}) = E(0) + \frac{\hbar^2}{2}\left(\frac{k_x^2 + k_y^2 + k_z^2}{m^*}\right) \qquad m^* = 0.067\, m_0$$



A better approximation is the non-parabolic expression:

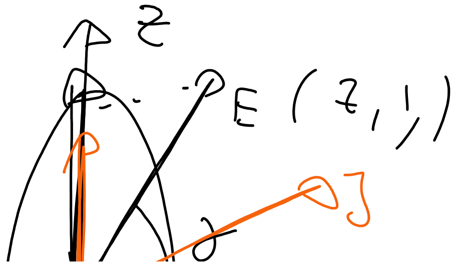
$$E(1 + \alpha E) = \frac{\hbar^2 k^2}{2 m^*}$$

With $\alpha = 0.67\, eV^{-1}$

Effective mass tensor → conductivity

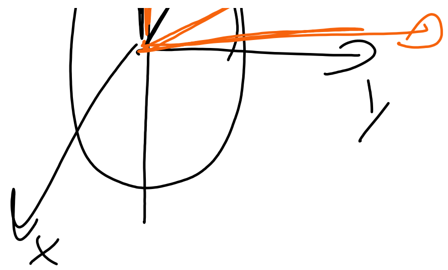
μ_e　　$\vec{V}_d = \mu_e \vec{E}$　　$\mu = \dfrac{q\,\tau_s}{m^*}$

Si



$E_t = E \cos\vartheta$

$E_\ell = E \sin\vartheta$

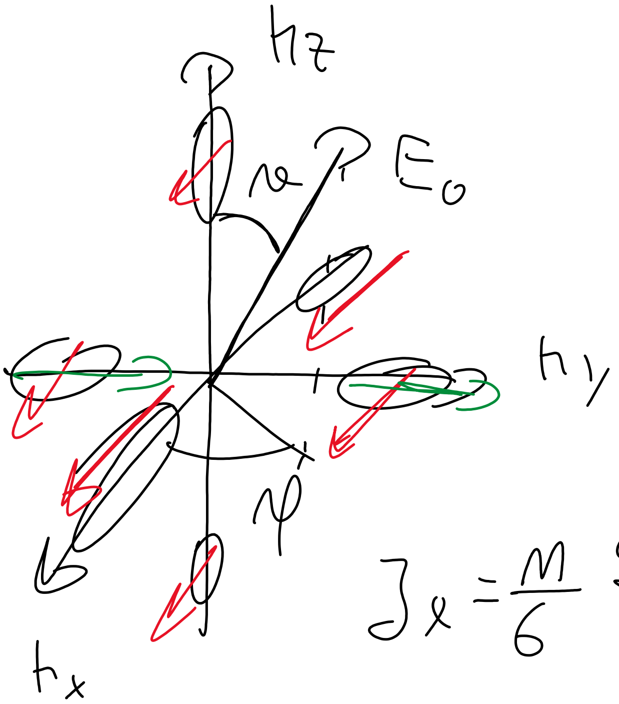


$$V_t = \frac{g \tau_s}{m_t} E \cos\alpha$$

$$V_\ell = \frac{g \tau_s}{m_\ell} E \sin\alpha$$

$$\underline{J} = n g V_d \nearrow J_t \quad \searrow J_\ell$$

$$n \left(\frac{e\ell}{cm^3} \right) \rightsquigarrow$$



$$E_x = E_0 \sin\vartheta \cos\varphi$$

$$E_y = E_0 \sin\vartheta \sin\varphi$$

$$E_z = E_0 \cos\vartheta$$

$$J_x = \frac{n}{6} g^2 \tau_s \left(\frac{2}{m_\ell} + \frac{4}{m_t} \right) \underline{E_x}$$

$$= \frac{n}{3} g^2 \tau_s \left(\frac{1}{m_\ell} + \frac{2}{m_t} \right) E_x$$

$$J_y = \frac{n}{3} g^2 \tau_s \left(\frac{1}{m_\ell} + \frac{2}{m_t} \right) \underline{E_y}$$

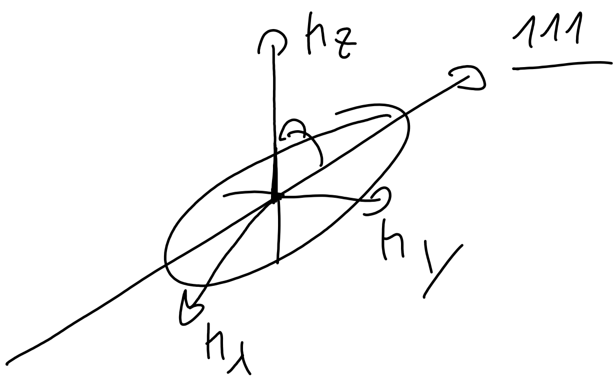
$$J_z = \quad '' \quad\quad ''$$

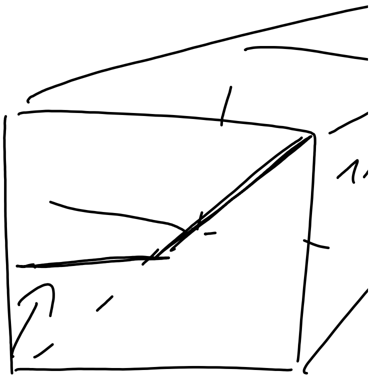
$$J = n g^2 \tau_s \quad\quad 1 \quad - \quad 1 \left(1 \quad + \right.$$

$\ldots y \qquad \frac{1}{m^*} \qquad \frac{1}{m^*_\sigma} = \frac{1}{3}\left(\frac{1}{m_e} + \ldots\right.$

$Si \rightarrow \frac{1}{m^*_\sigma} = 0{,}26$

$Ge \rightarrow \frac{1}{m^*_\sigma} = 0.12$



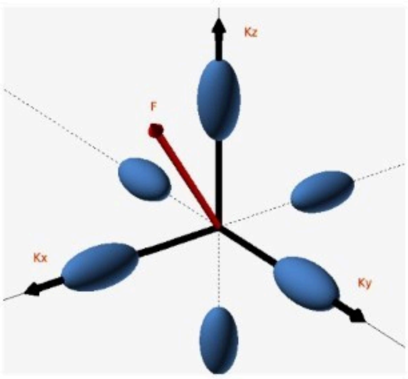


$[1\ -1\ 0] \cdot [1\ 1\ \ldots$

$[1\ 1\ 1] \times [1\ -1\ \ldots$

$\frac{[0\,0\,1] \cdot [1\,1\,1]}{\sqrt{3}} = \cos\theta \qquad [0\,0\,1]$

Conductivity effective mass in Si



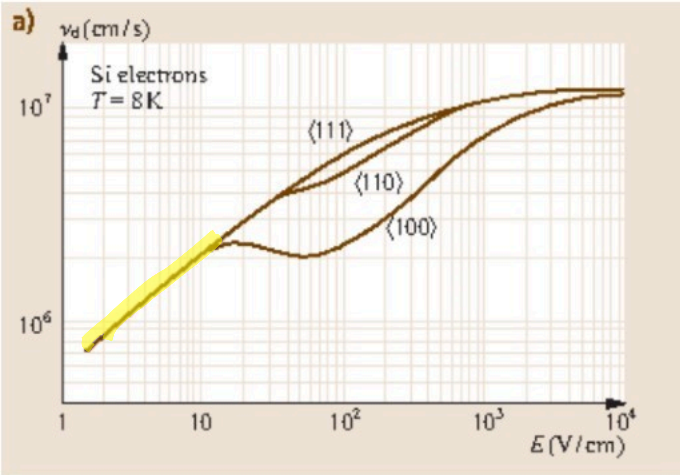
$$J_x = q\frac{n}{3}\left(2\frac{q\tau}{m_t} + \frac{q\tau}{m_l}\right)F_x,$$
$$J_y = q\frac{n}{3}\left(2\frac{q\tau}{m_t} + \frac{q\tau}{m_l}\right)F_y,$$
$$J_z = q\frac{n}{3}\left(2\frac{q\tau}{m_t} + \frac{q\tau}{m_l}\right)F_z.$$

$$\sigma = q^2\tau n\,\frac{1}{3}\left(\frac{2}{m_t} + \frac{1}{m_l}\right) \qquad \frac{1}{m_c} = \frac{1}{3}\left(\frac{2}{m_t} + \frac{1}{m_l}\right)$$

Hot-electrons effects in silicon

Anisotropic conduction is observed at high electric field E due to valley re-population

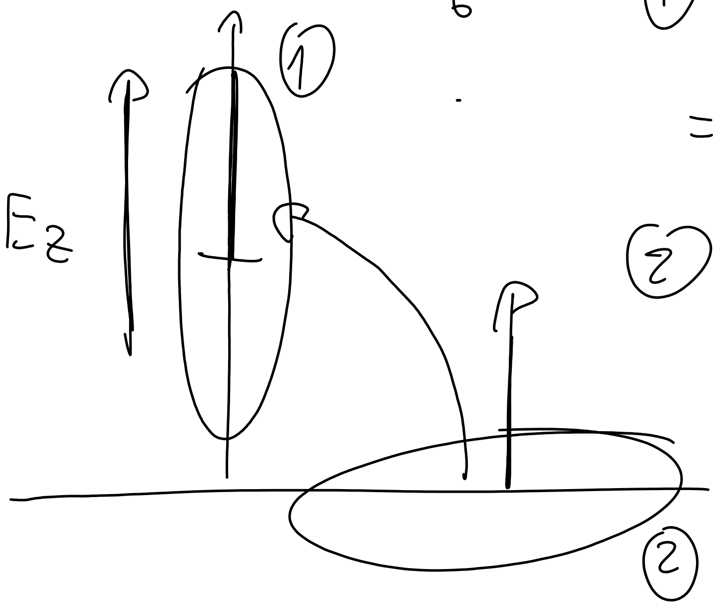
when E ‖ ⟨ 111 ⟩ the six valleys are equally oriented with respect to F and all of them give the same contribution to the drift velocity v_d. When E ‖ ⟨ 100 ⟩, two valleys exhibit the effective mass m_l in the direction of the field, while the remaining four exhibit the transverse mass $m_t < m_l$. Electrons in the transverse valleys respond with a higher mobility, are heated to a greater extent by the field and transfer electrons to the two longitudinal, colder and slower valleys, which results in a lower v_d than for E ‖ ⟨ 111 ⟩, as seen in the figure



$\vec{J} = \sigma \vec{E}$ $\qquad \sigma = n \dfrac{q^2 \tau_s}{m^*_\sigma}$

n_z

$\vec{J} \cdot \vec{E}$



① $E_z \cdot J_z = E_z \cdot$

$= E_z^2 \cdot \dfrac{n}{6} \dfrac{q^2 \tau_s}{m_e}$

② $E_z^2 \cdot \dfrac{n}{6} \dfrac{q^2 \tau_s}{m_t}$

$n_{1/}$

Power

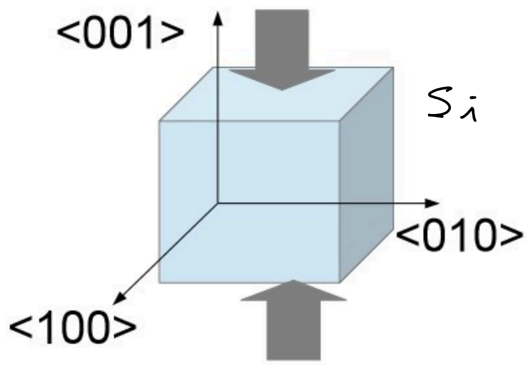
Z-VALLEY

Denisty of states and conductivity effective mass

See Appendix A.2 “SemiconductorNanostructures.pdf”

COMPRESSIVE STRESS (001)

G= conductivity



$G/G_0=0.433$

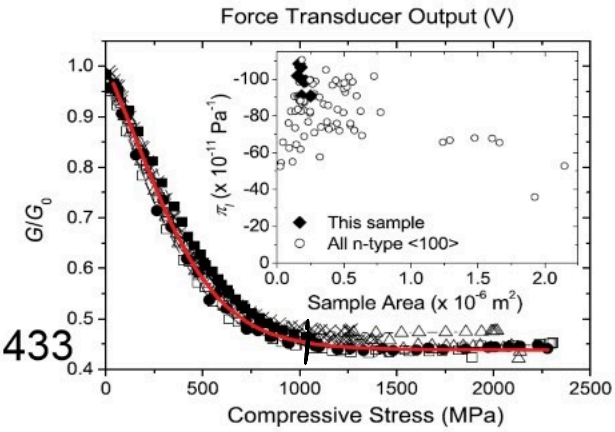
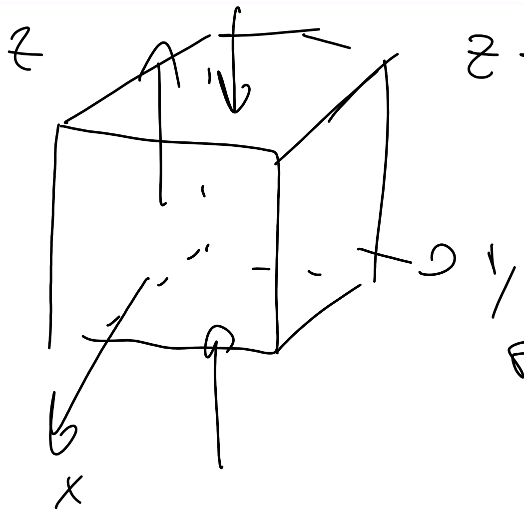
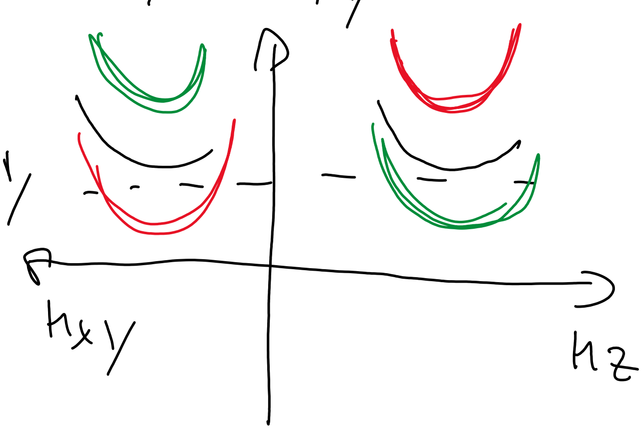


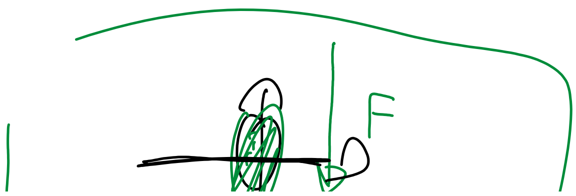
FIG. 2 (color online). (a) Raw data obtained for X parallel to the ⟨100⟩ crystal direction in n-type silicon, showing discontinu-

Phys. Rev. Lett. 108, 256801 (2012)

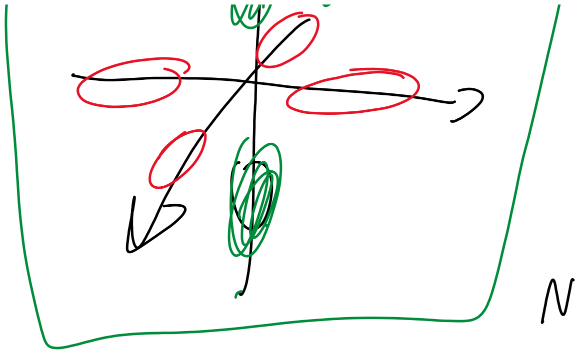


z → ≠ x, y





$J_z = \frac{m}{\dots} \frac{q^2 \tau}{\dots} \left(\frac{2}{m \dots} \right) =$



$$= \frac{n g^2 \tau_s}{m_e}$$

$$\text{No-strain} = n g^2 \tau \, \frac{1}{3}\left(\frac{2}{m_t} + \frac{1}{m_e}\right)$$

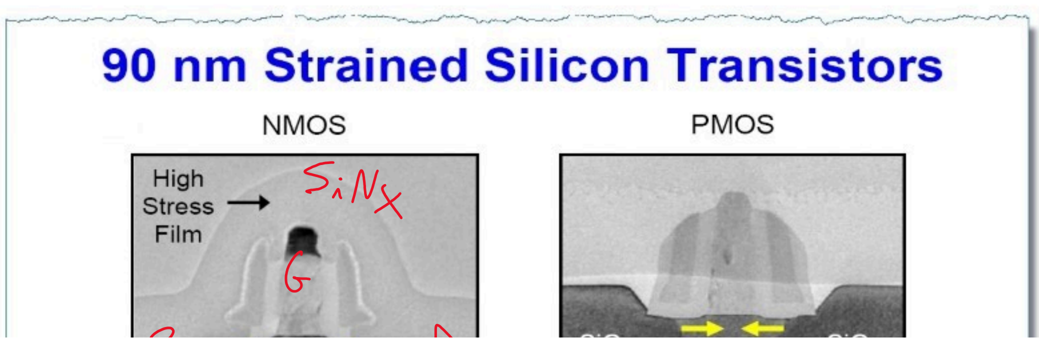
$$\frac{\sigma}{\sigma_0} = 0{,}43 = \frac{\dfrac{\cancel{n}\,\cancel{g^2}\,\tau_s}{m_e}}{\cancel{n}\,\cancel{g^2}\,\tau\,\frac{1}{3}\left(\frac{2}{m_t} + \frac{1}{m_e}\right)} = \frac{\tau_s}{\tau}\,\frac{\frac{1}{m_e}}{\frac{1}{3}\left(\ldots\right)}$$

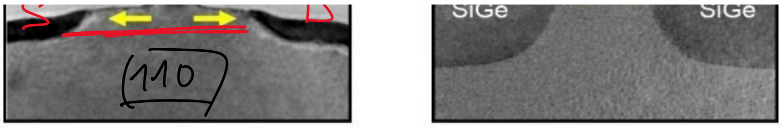
Si: $m_t = 0{,}19 \quad m_e = 0{,}98$

$$\frac{\tau_s}{\tau} = \frac{\sigma}{\sigma_0} \cdot \frac{\frac{1}{3}\left(\frac{2}{m_t} + \frac{1}{m_e}\right)}{\frac{1}{m_e}} = 0{,}43 \cdot 3{,}8$$

$$\tau_s = 1.6\,\tau$$

Strained silicon technology-uniaxial strain





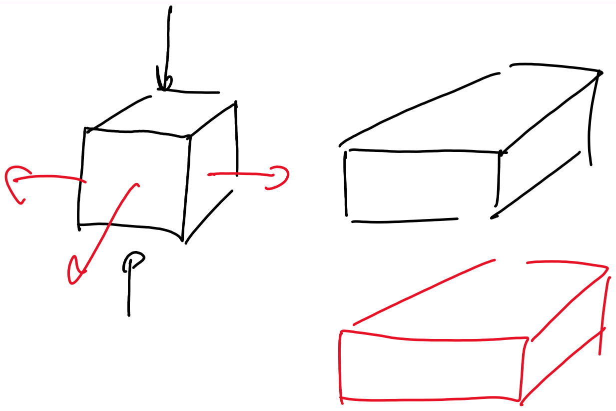
SiN cap layer
Tensile channel strain

SiGe source-drain
Compressive channel strain

NMOS strain was created by adding a high-stress layer that wrapped around the transistor. PMOS strain was created by replacing the conventional source/drain region with strained SiGe

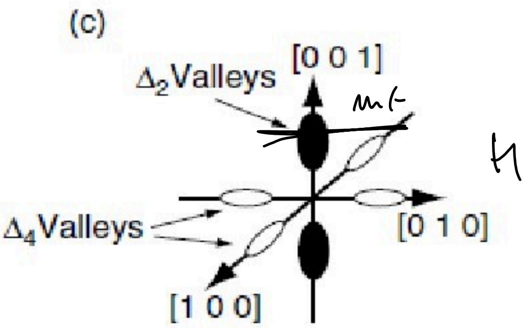
intel

C. Auth, VLSI 2008



COMPRESSIVE
ALONG
001
||
TENSILE STRESS
ALONG
100 / 010

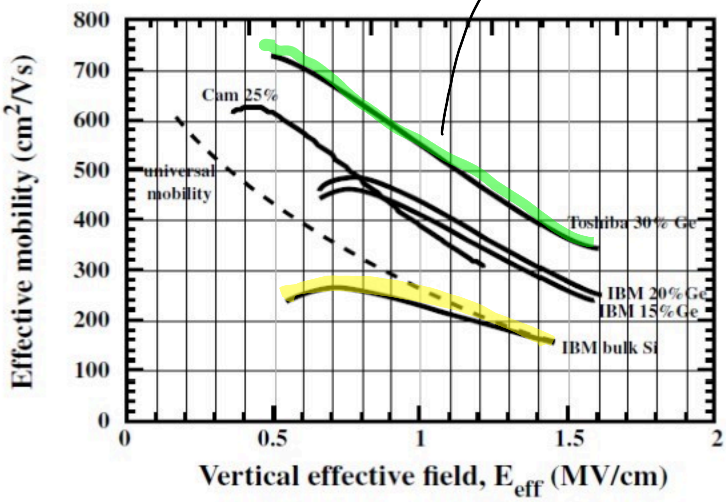
Strained silicon technology-uniaxial strain



H

N-MOS

$$\mu = \frac{q \tau_s}{m_t}$$



$m_e, m_t \rightarrow m^*_d$

$\rightarrow$ DOS (3D) $= \frac{\sqrt{2}}{\pi^2 \hbar^3} (m^*)^{3/2} \sqrt{E}$

$$E = \frac{\hbar^2 k_e^2}{2 m_e} + \frac{\hbar^2 k_t^2}{2 m_t} + \frac{\hbar^2 k_t^2}{2 m_t} \qquad \frac{x^2}{a^2} + \frac{}{}$$

$$\text{Volume} = \frac{4}{3} \pi a b c \qquad a = \frac{\sqrt{2 m_e}}{\hbar}$$

$$V_k = \frac{4}{3} \pi 2^{3/2} \sqrt{m_e m_t^2} E^{3/2}$$

SPIN

$$\frac{\text{NUMBER STATES}}{\text{VOLUME } (cm^3)} = \frac{V_k}{\left(\frac{2\pi}{L}\right)^3} \times 2 \frac{1}{L^3} = \frac{1}{3\pi}$$

L = "CUBE" SIDE

IN REAL SPACE

DOS $\Rightarrow$ $\frac{\text{NUMBER OF STATES}}{\text{VOLUME Energy}}$ $\rightarrow$

3

$$DOS = \frac{1}{3\pi^2 \hbar^3} 2^{3/2} \sqrt{m_e m_t^2} \frac{d E^{3/2}}{dE}$$

$$DOS = \frac{\sqrt{2}}{\pi \hbar^3} \sqrt{m_e m_t^2} \sqrt{E} \times M$$

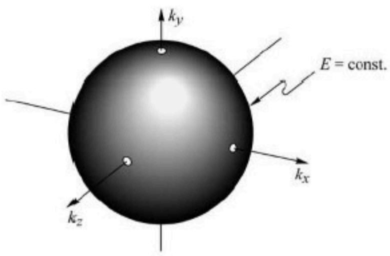
$$\frac{\sqrt{2}}{\pi \hbar^3} m_*^{3/2} \sqrt{E}$$

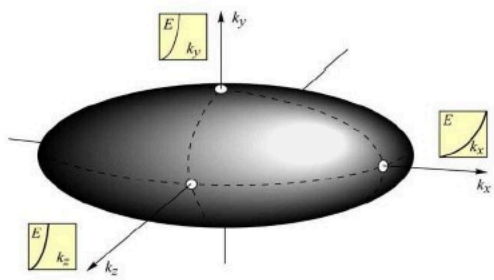
$$m_*^{3/2} = (m_e m_t^2)^{1/2} \rightarrow m_* = \sqrt[3]{\,}$$

$$m_{DOS}^{3/2} = M (m_e m_t^2)^{1/2}$$

$$m_{DOS} = M^{2/3} \sqrt[3]{m_e m_t^2}$$

The density of state effective mass





$$E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m^*}$$

$$\frac{x^2}{a^2}+\frac{y^2}{b^2}+\frac{z^2}{c^2}=1 \qquad V = 4/3\,\pi abc$$

$$\frac{k_x^2}{2m_x E/\hbar^2}+\frac{k_y^2}{2m_y E/\hbar^2}+\frac{k_z^2}{2m_z E/\hbar^2}=1$$

$$DOS = \frac{\sqrt{2}}{\pi^2\hbar^3} m_{DOS}^{3/2}\sqrt{E}$$

$$\text{DOS} = M\times\frac{\sqrt{2}}{\pi^2\hbar^3}\sqrt{m_x m_y m_z}\sqrt{E}$$

$$m_{DOS} = M^{3/2}\left(m_x m_y m_z\right)^{1/3}$$

Denisty of states and conductivity effective mass

Table 0-2. Effective mass and energy bandgap of Ge, Si and GaAs

Name	Symbol	Germanium	Silicon	Gallium Arsenide
Smallest energy bandgap at 300 K	E_g (eV)	0.66	1.12	1.424
Effective mass for density of states calculations				
Electrons	$m_{e,dos}^*/m_0$	0.56	1.08	0.067
Holes	$m_{h,dos}^*/m_0$	0.29	0.57/0.81[1]	0.47
Effective mass for conductivity calculations				
Electrons	$m_{e,cond}^*/m_0$	0.12	0.26	0.067
Holes	$m_{h,cond}^*/m_0$	0.21	0.36/0.386 [7]	0.34

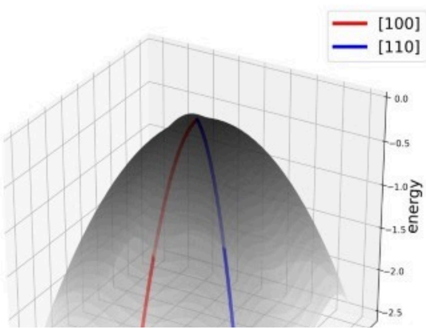
$m_0 = 9.11 \times 10^{-31}$ kg is the free electron rest mass.

Hole effective mass

$$E_{HH} = -\frac{1}{2m_0}\left(Ap^2 + \sqrt{B^2p^4 + C^2\left(p_x^2p_y^2 + p_y^2p_z^2 + p_z^2p_x^2\right)}\right)$$

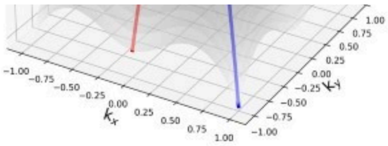
$$E_{LH} = -\frac{1}{2m_0}\left(Ap^2 - \sqrt{B^2p^4 + C^2\left(p_x^2p_y^2 + p_y^2p_z^2 + p_z^2p_x^2\right)}\right)$$

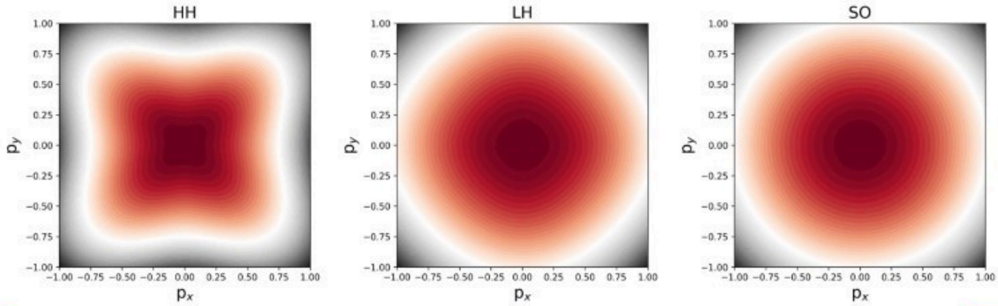
$$E_{SO} = -\Delta_0 - \frac{1}{2m_0}Ap^2,$$



	Si	Ge

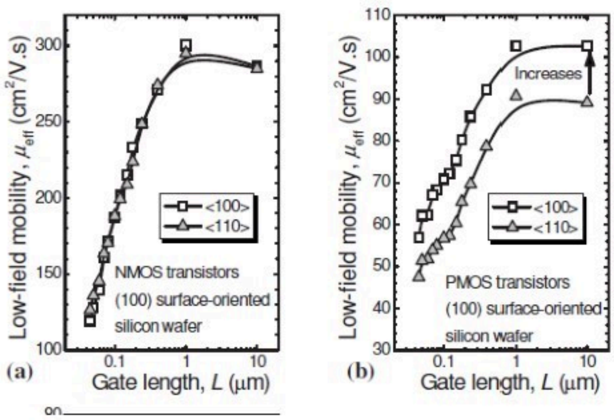
Δ_0	0.044 eV	0.29
A	-4.0±0.2	-13.3±0.2
B	±1.1±0.2	±8.6±0.1
C	±4.1±0.5	±12.5±0.2





Effective mass in n and p MOS

In Si the electron conductivity mass is isotropic i.e. the mobility does not depend on the direction of current flow (see left panel).
On the other hand, the hole effective mass is highly anisotropic. Looking at the isoenergetic contour on the previous slide we notice that the HH effective mass is larger along <110> and smaller along <100>. As a results the hole mobility will be higher along <100> (right panel).



Electrons and holes effective mass

Electron effective mass

Material	el. eff.	Bandgap

Hole effective mass

Material	Hole eff.

	mass	(eV)
GaAs	0.063	1.42
InP	0.077	1.35
GaSb	0.042	0.72
InAs	0.023	0.36
InSb	0.0145	0.17

Semiconductors for high electron mobility transistors
GaAs, InGaAS, InP, InGaP

	mass
Si	0.16 0.49
Ge	0.04 0.28
GaAs	0.076 0.5
InP	0.64
GaSb	0.40
InAs	0.40
InSb	0.40