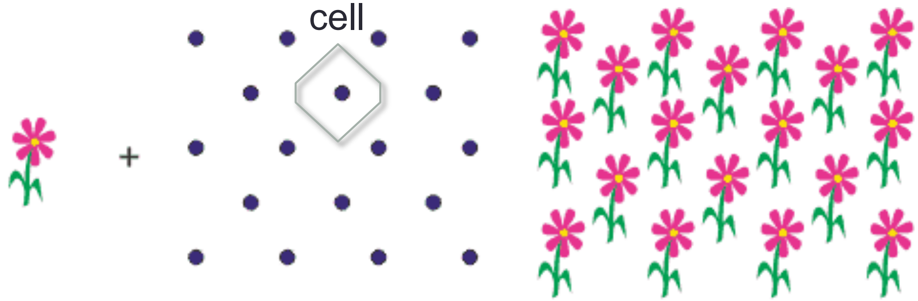
MOBILITIES IN GERMANIUM

Bart Bruyneel
CEA Saclay, France
05-09/12/2011 EGAN school, Liverpool

Intro

Real World

Wigner-Seitz cell

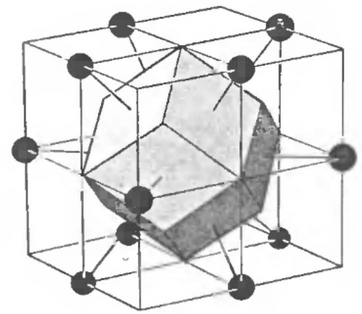


Primitive cell

+ Bravais Lattice **"R"**

= Crystal

Monocrystalline Ge



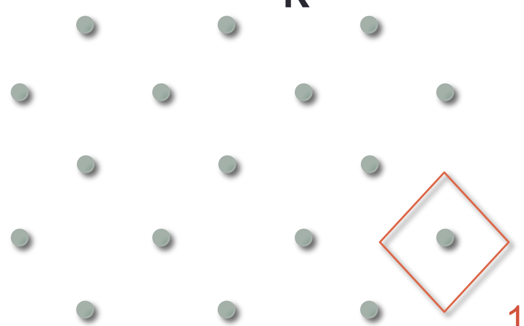
"Face centered cubic"

FT

Fourier transform

K – Space

Reciprocal Lattice **"K"**

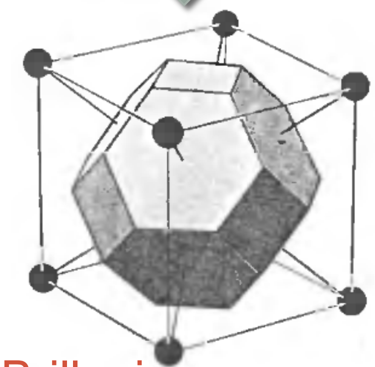


1st Brillouin zone

= All wave vectors with periodicity of the lattice

$$e^{i\vec{K}\cdot\vec{R}} = 1$$

FT



1st Brillouin zone = "Body centered cubic"

Bloch's theorem

The eigenstates of the Hamiltonian $H\Psi = \left(-\frac{\hbar^2}{2m}\Delta + U(\vec{r})\right)\Psi = \varepsilon\Psi$

Where $U(\vec{r}+\vec{R}) = U(\vec{r})$ for all R in the Bravais lattice, can be chosen in the form of a plane wave times a function with periodicity of the Bravias lattice:

$$\boxed{\Psi_{n,k} = e^{i\vec{k}\cdot\vec{r}} u_{n,\vec{k}}(\vec{r})}$$

Properties:

- $\Psi_{n,\vec{k}}$ and $\varepsilon_n(\vec{k})$ are periodic in k space:

$$\Psi_{n,\vec{k}+\vec{K}} = \Psi_{n,\vec{k}}$$

$$\varepsilon_n(\vec{k}+\vec{K}) = \varepsilon_n(\vec{k})$$

➔

- all distinct values of $\varepsilon_n(\vec{k})$ occur for **k**-values in the first Brillouin zone

- Energies $\varepsilon_n(\vec{k})$ for fixed n vary continuously with **k**
  ➔ n = *band index*

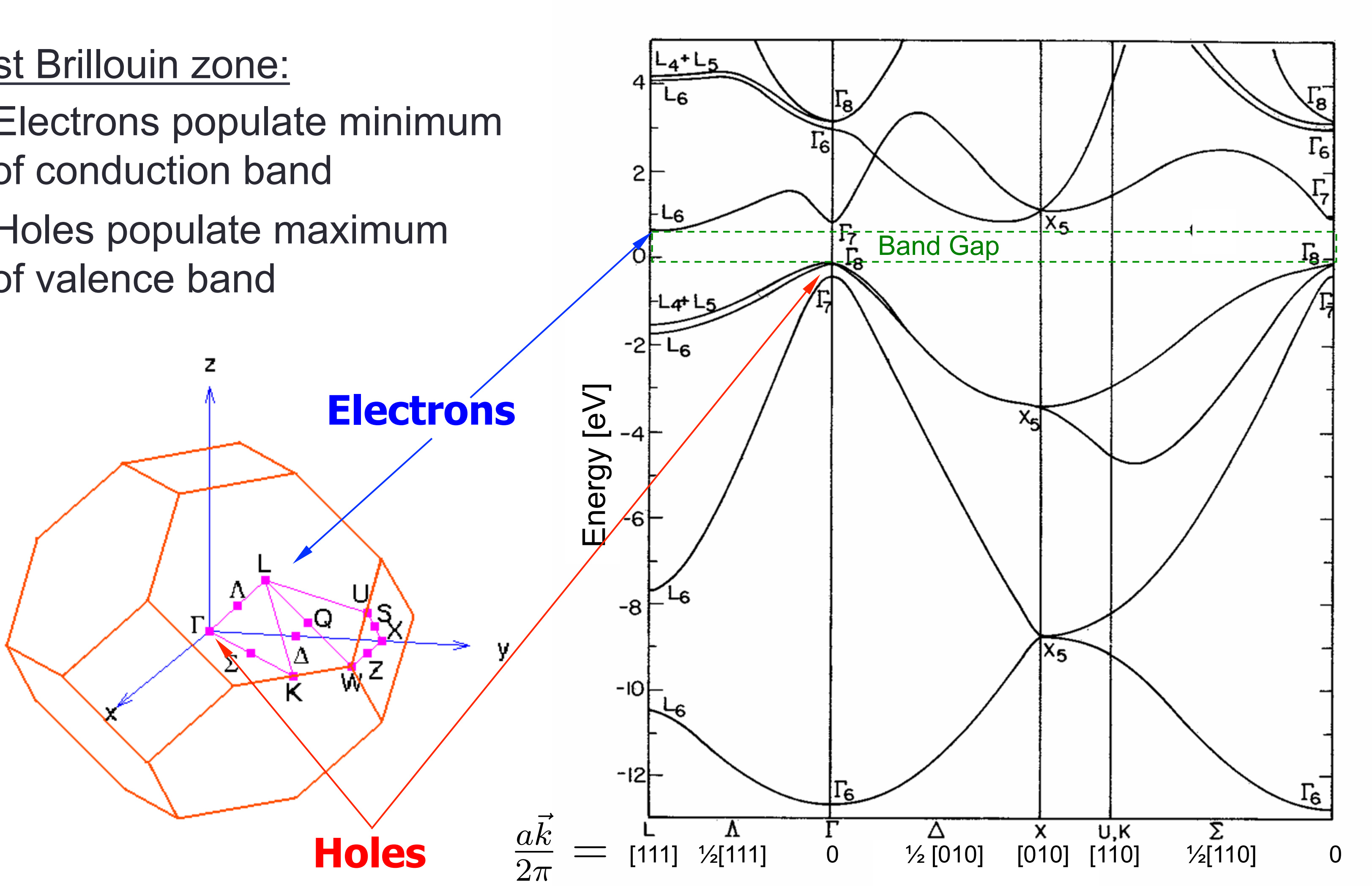
- Group **velocity v**:

$$\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}}\varepsilon_n(\vec{k})$$

Germanium Band structure

first Brillouin zone:

- Electrons populate minimum of conduction band
- Holes populate maximum of valence band



Anisotropic Mobility

- Often neighborhood of valence band is quadratic (+ for electrons / - for holes).

$$\varepsilon(\vec{k}) = \varepsilon_c \pm \frac{\hbar^2}{2} \sum_{\mu,\nu} k_\mu (\mathbf{M^{-1}})_{\mu,\nu} k_\nu$$

- By choosing appropriate principle axis, mass tensor M becomes diagonal:

$$\varepsilon(\vec{k}) = \varepsilon_c \pm \frac{\hbar^2}{2} \left(\frac{k_1^2}{m_1} + \frac{k_2^2}{m_2} + \frac{k_3^2}{m_3} \right)$$

- ➔Group velocity:

$$\vec{v}(\vec{k}) = \frac{1}{\hbar} \vec{\nabla}_{\vec{k}} \varepsilon_n(\vec{k}) = \pm\hbar \left(\frac{k_1}{m_1}, \frac{k_2}{m_2}, \frac{k_3}{m_3} \right)$$

- Drift velocity is average over population of levels:

$$\vec{v}_d = \iiint \vec{v}(\vec{k}) f(\vec{k}) d\vec{k}$$

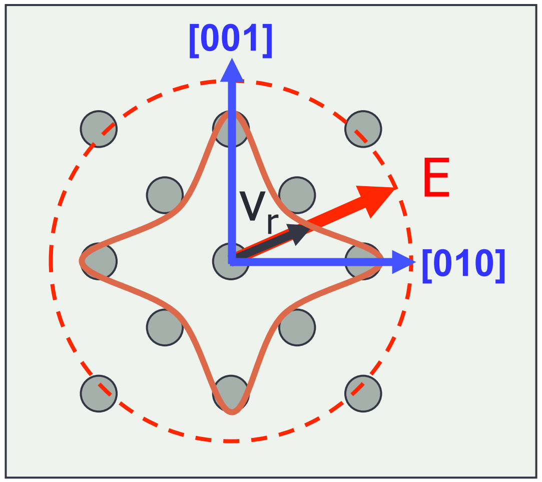
- Distribution f(k) found by solution of Boltzman equation as balance between variation due to field and variation due to scattering
  scattering = interaction with phonons, impurities, defects, other carriers

Anisotropic Mobility

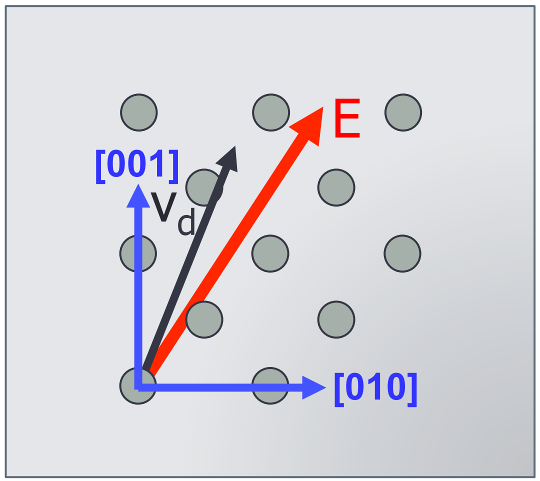
$$\vec{v}_d = \iiint \vec{v}(\vec{k}) f(\vec{k}) d\vec{k}$$

- At high fields, radial anisotropy is observed
- Radial anisotropy induces tangential anisotropy: a drift component towards the faster axis
- For fields along symmetry axis, no tangential drift components can exist: Crystal + E field are then invariant under certain rotations; so must be the drift

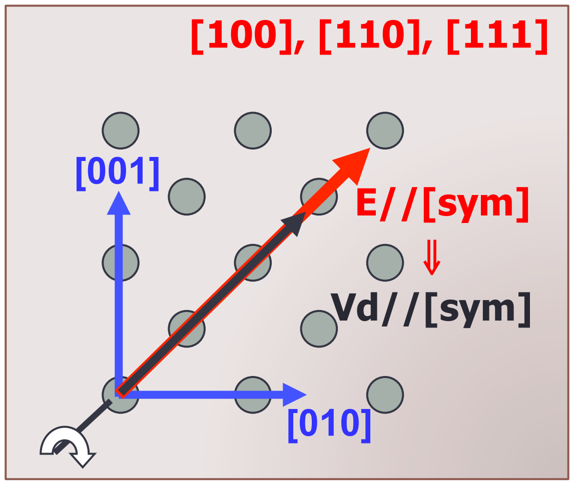
Radial anisotropy,



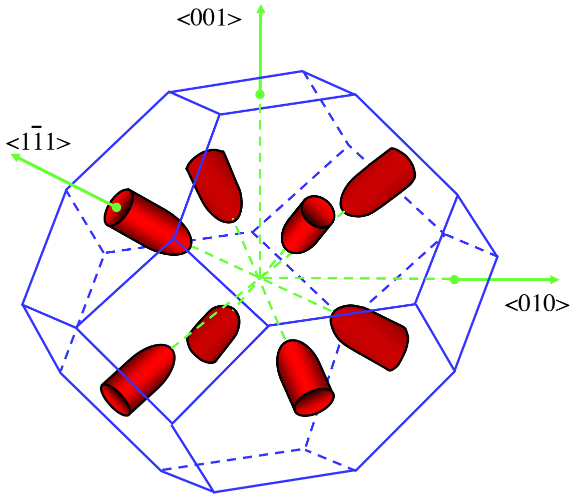
Tangential anisotropy,



except for E // symmetry axis



Germanium – Electron mobility



- Electrons distributed over 4 ellipsoidal valleys
  $\vec{v}_d = \sum_{i=1}^{4} n_i \vec{v}_i$
- Linear transf. $\vec{k}^* = \alpha_i^{1/2} \vec{k}$ makes valley i spherical:
  with R_i appropriate rotation matrices

$$\alpha_i = R_i^T \cdot \begin{pmatrix} m_t^{-1} & 0 & 0 \\ 0 & m_l^{-1} & 0 \\ 0 & 0 & m_t^{-1} \end{pmatrix} \cdot R_i$$

- In $\vec{k}^*$ space, the mobility is isotropic: $\vec{v}_i^*(\vec{E}) = -\mu^*(E_i^*)\vec{E}_i^*$
  with μ^* a **scalar** function of *E**
- The field and velocities transform as: $\vec{E}_i^* = \alpha_i{}^{1/2} \vec{E}$ and $\vec{v}_i^* = \alpha_i{}^{-1/2} \vec{v}$

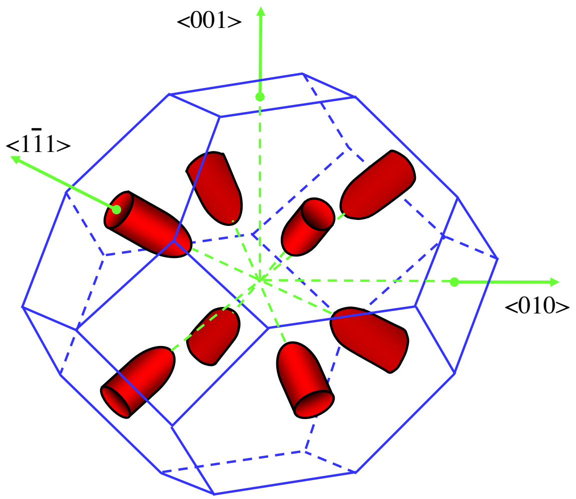
- Filling everything in yields:

$$\boxed{\vec{v}_d(\vec{E}) = -\sum_{i=1}^{4} n_i \, \mu^*(E_i^*) \, \alpha_i \vec{E}}$$

Phys.Rev. 130(6):2201-2204 (1963)

NIM A. 447 (2000) 350-360

Germanium – Electron mobility



$$\vec{v}_d(\vec{E}) = -\sum_{i=1}^{4} n_i\, \mu^*(E_i^*)\, \alpha_i \vec{E}$$

- If E // <100> : n_i= ¼, and

$$\alpha_i \vec{E} = \Gamma_0 E_x \vec{e}_x \qquad \Gamma_0 = 2.888$$

$$\boxed{\mu^*(E) = \frac{v_{100}(E/\Gamma_0)}{\Gamma_0 E}}$$

- Population of each valley is defined by intervalley scattering rate ν
  In equilibrium state:

$$\boxed{n_i = \frac{\nu(E_i^*)^{-1}}{\sum_{k=1}^{4} \nu(E_k^*)^{-1}}}$$

Germanium – Electron mobility

Summary:

- v_{100} drift velocity defines μ^*
- Intervalley scattering rate defines n_i

$$\vec{v}_d(\vec{E}) = -\sum_{i=1}^{4} n_i\, \mu^*(E_i^*)\, \alpha_i \vec{E}$$

Parametrization:

- $\nu(E) \propto E^\eta$ with $\eta(E) = \eta_0 + \eta_1 \log E/E_0 + \eta_2 (\log E/E_0)^2$
  Parameters can be obtained by fit to v_{111} and/or v_{110} drift velocity data

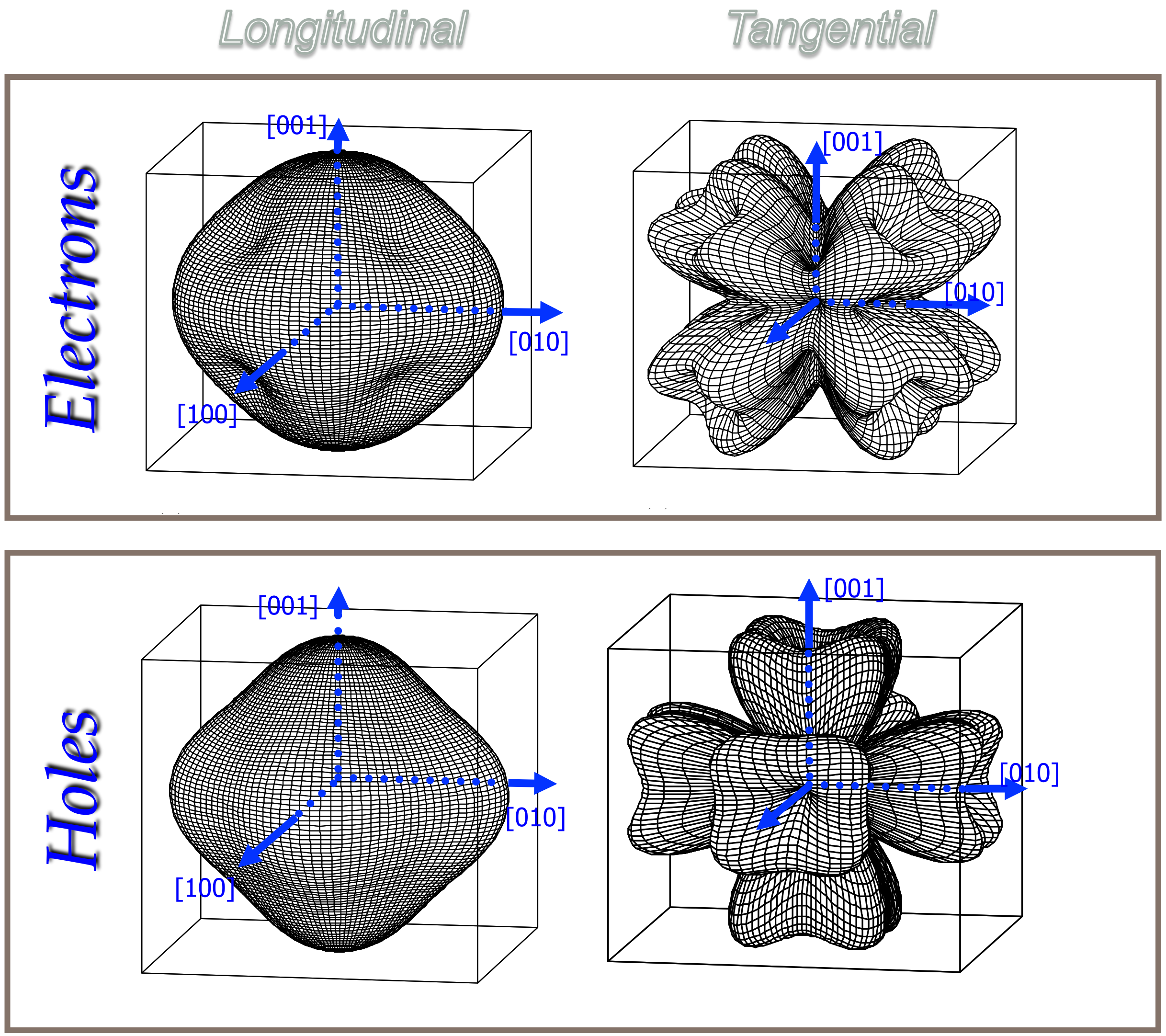
- $v_{100} = \dfrac{\mu_0 E}{(1 + (\frac{E}{E_0})^\beta)^{\frac{1}{\beta}}} - \mu_n E$

Parameters currently used in ADL:

- See file “Template_DRIFT_GE.txt”

```
#Electron Mobility Parameters:
#Mobility in 100:
ADL_G_E0e100            507.7
ADL_G_Be100             0.80422
ADL_G_Mu0e100           0.0371654
ADL_G_MuNe100           -0.0001447
#Intervalley Scattering rate:
ADL_G_LnNu0             0.459
ADL_G_LnNu1             0.0294
ADL_G_LnNu2             0.000054
ADL_G_E0                1200.0
```

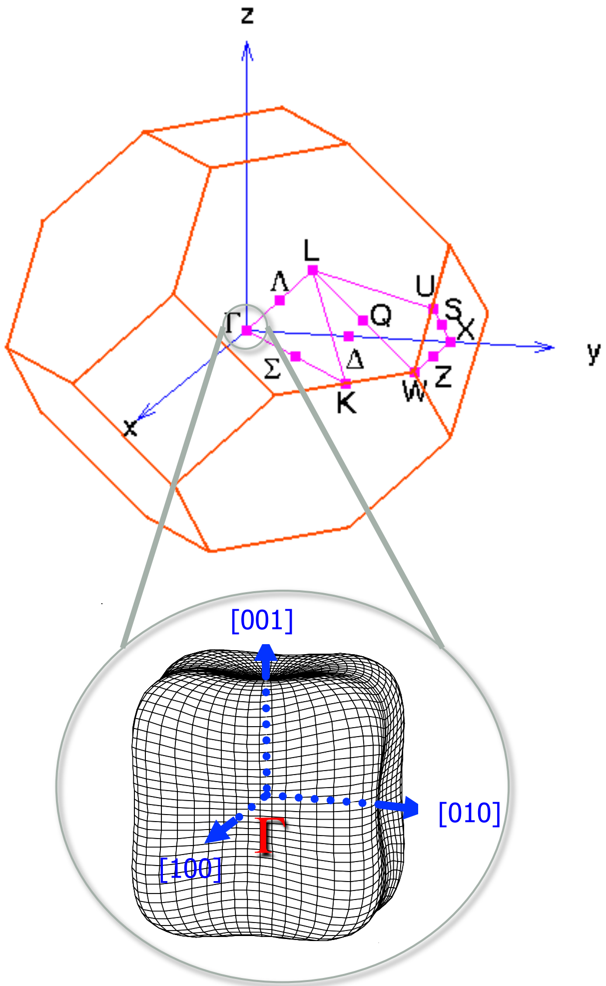
Anisotropy in mobility



- Longitudinal and tangential components of drift velocity as function of orientation of the field (1200 V/cm)

- Electrons v_r mainly slower near [111],
- Holes v_r mainly faster near [100]
- Tangential components:
  -0 along symmetry axes
  -pointing towards nearest [100] axis

Germanium – Hole mobility

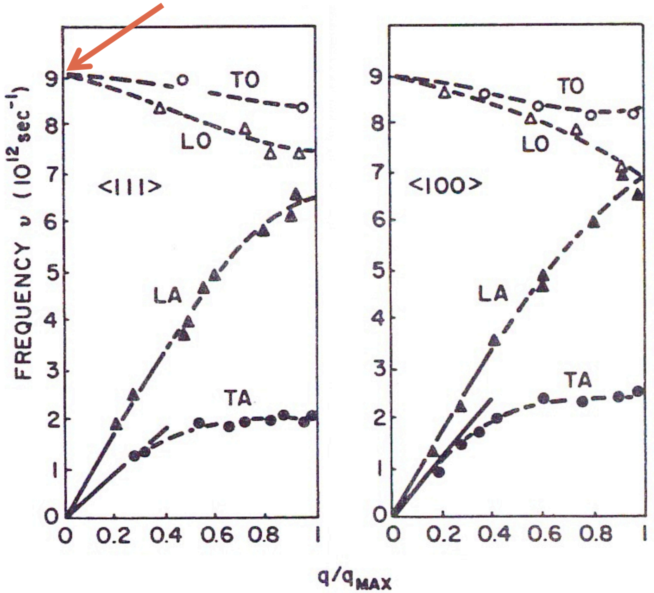


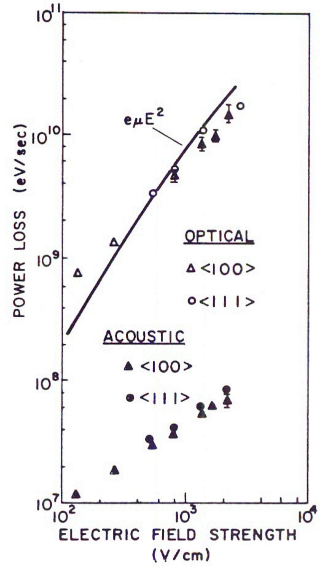
- Maximum of conduction band in middle of 1st brillouin zone
- Band structure there is 2-fold degenerate into a heavy ($0.3m_0$) and a light hole ($0.04m_0$) band.
- Light hole band can be neglected due to smaller density of states
- Next band is 0.29eV lower : not accessible (see streaming motion model)

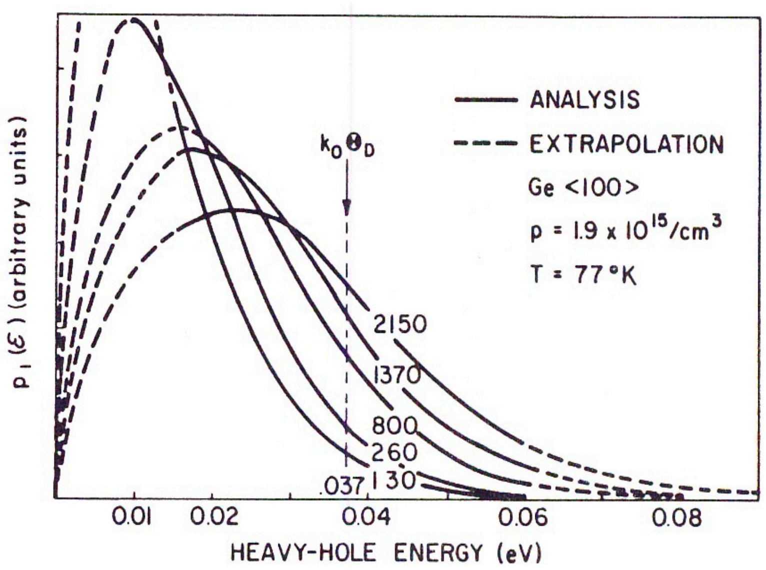
- **<u>Streaming motion:</u>**
  - energy loss by acoustic phonons is negligible
  - holes accelerate up to 0.037eV, then
  - optical phonon emission is very likely.
  - the hole loses all its energy in this
  - the streaming motion is repeated

Germanium & phonons

0.037eV







Proof for streaming motion picture
and Drifted Maxwellian distribution

pictures taken from:
E. M. Conwell, High field transport in semiconductors, Solid State Physics 9 (1967).

Germanium – Hole mobility

Ingredients in the model:

- Drifted Maxwell-Boltzman distribution

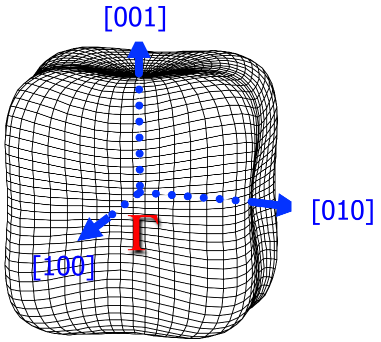
$$f(\vec{k};\vec{k}_0) = a \cdot \exp(-\hbar^2(\vec{k}-\vec{k}_0)^2/2mk_bT_h) \quad \text{with} \quad \vec{k}_0 // \vec{E}$$

- Warped heavy hole band

$$\epsilon(\vec{k}) = A \cdot \frac{\hbar^2 k^2}{2m_0} \cdot [1 - q(\theta,\phi)]$$

$$q(\theta,\phi) = [b^2 + \frac{c^2}{4} \cdot (\sin(\theta)^4 \sin(2\phi)^2 + \sin(2\theta)^2)]^{1/2}$$

$A = 13.35 \qquad b = 0.6367 \text{ and } c = 0.9820$



Germanium – Hole mobility

- Approximate solution to $\vec{v}_d = \frac{\hbar}{a\pi^{3/2}\sqrt{2mk_bT_h}} \int \vec{v}(\vec{k})\, f(\vec{k};\vec{k}_0)\, d\vec{k}$:
- Let $\vec{E}(E,\theta_0,\phi_0)$, then

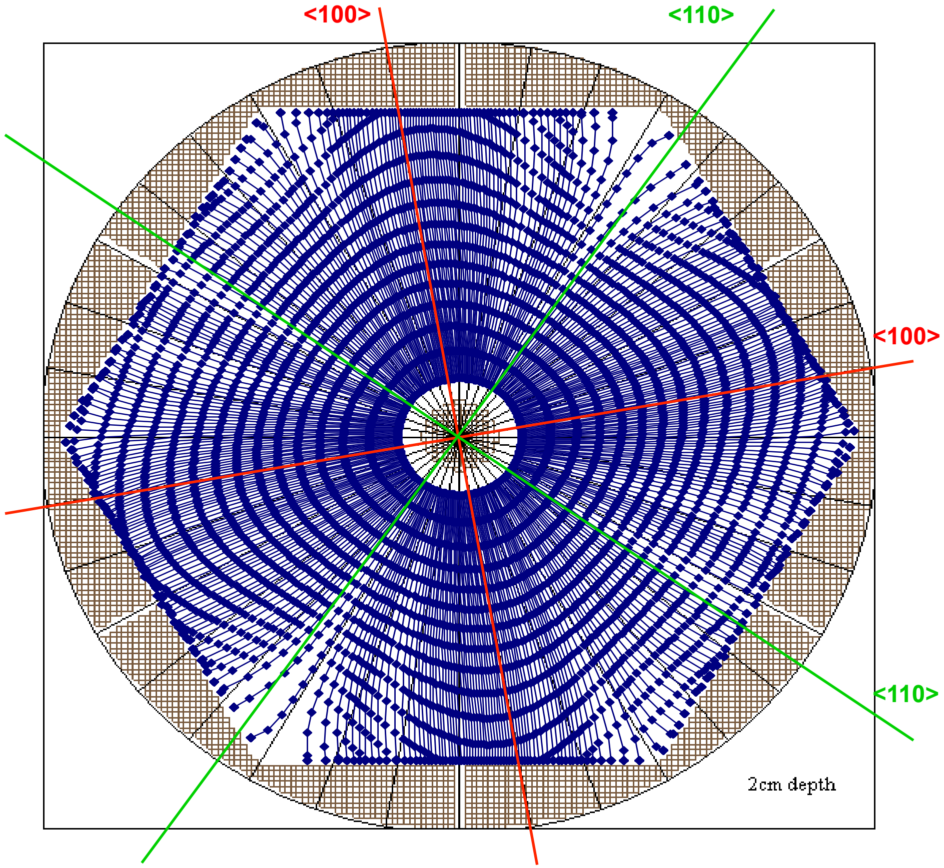
$$\boxed{\begin{aligned}
v_r &= v_{100}(E)[1 - \Lambda(k_0)(\sin(\theta_0)^4 \sin(2\phi_0)^2 + sin(2\theta_0)^2)] \\
v_\theta &= v_{100}(E)\Omega(k_0)[2\sin(\theta_0)^3 \cos(\theta_0)\sin(2\phi_0)^2 + \sin(4\theta_0)] \\
v_\phi &= v_{100}(E)\Omega(k_0) sin(\theta_0)^3 \sin(4\phi_0)
\end{aligned}}$$

- The Anisotropic “amplitudes” are given by

$$\Lambda(k_0) = -0.01322k_0 + 0.41145k_0^2 - 0.23657k_0^3 + 0.04077k_0^4$$
$$\Omega(k_0) = 0.006550k_0 - 0.19946k_0^2 + 0.09859k_0^3 - 0.01559k_0^4$$

- With k_0 from $k_0(v_{rel}) = 9.2652 - 26.3467v_{rel} + 29.6137v_{rel}^2 - 12.3689v_{rel}^3$ $\quad (v_{rel} = v_{111}/v_{100})$
- v100(E) and v111(E) determine model.

Example: Hole trajectories



Hole trajectories for homogeneous starting positions around the core electrode. Every 25ns a point was plotted on the trajectory

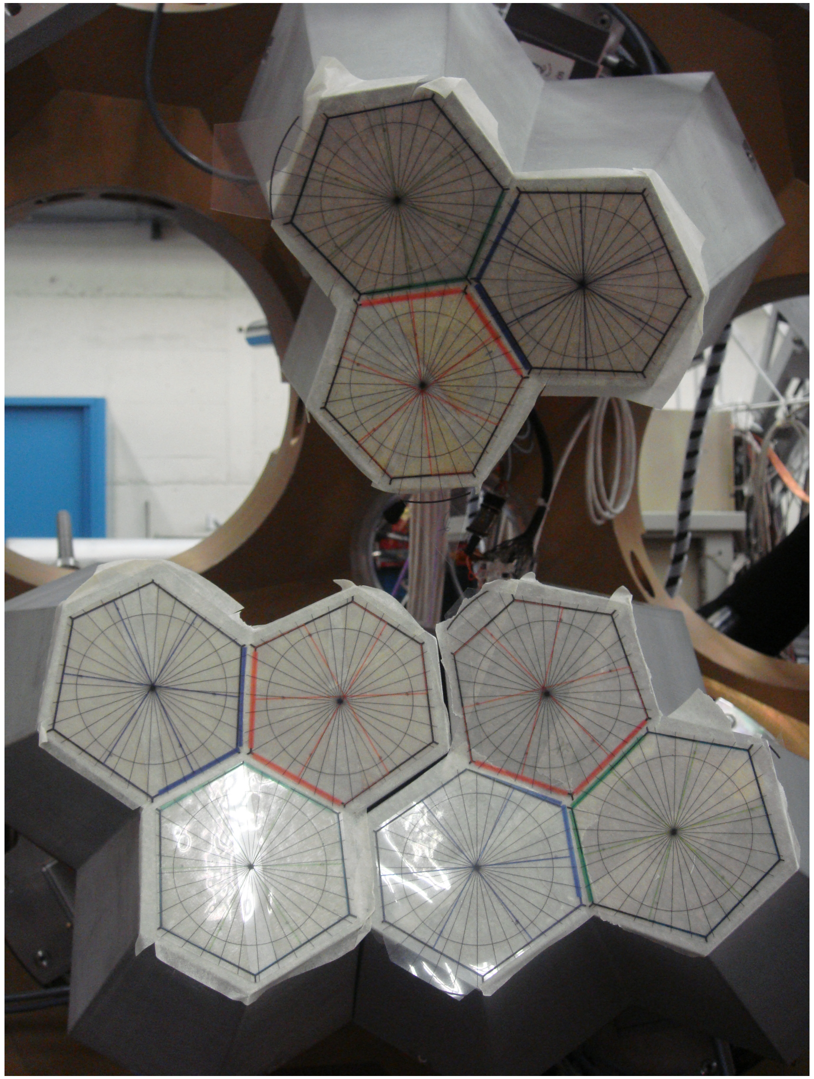
Parameters used in ADL:

Template_DRIFT_GE.txt

```
####################################################
#This file is an example for the setup of the file
#  ADL_DRIFT_GE
####################################################

#LATTICE ORIENTATION PARAMETERS:
ADL_G_LatticePhi          0.7853981633
ADL_G_LatticeTheta        0.0
ADL_G_LatticePsi          0.0

#Electron Mobility Parameters:
#Mobility in 100:
ADL_G_E0e100              507.7
ADL_G_Be100               0.80422
ADL_G_Mu0e100             0.0371654
ADL_G_MuNe100             -0.0001447
#Inter-valley Scattering rate:
ADL_G_LnNu0               0.459
ADL_G_LnNu1               0.0294
ADL_G_LnNu2               0.000054
ADL_G_E0                  1200.0

#Hole Mobility Parameters:
#Mobility in 100:
ADL_G_E0h100      181.9
ADL_G_Bh100       0.73526
ADL_G_Muh100      0.062934
#Mobility in 111:
ADL_G_E0h111      143.9
ADL_G_Bh111       0.7488
ADL_G_Muh111      0.062383

#Other Parameters:
ADL_G_SmallField          1e-6
```

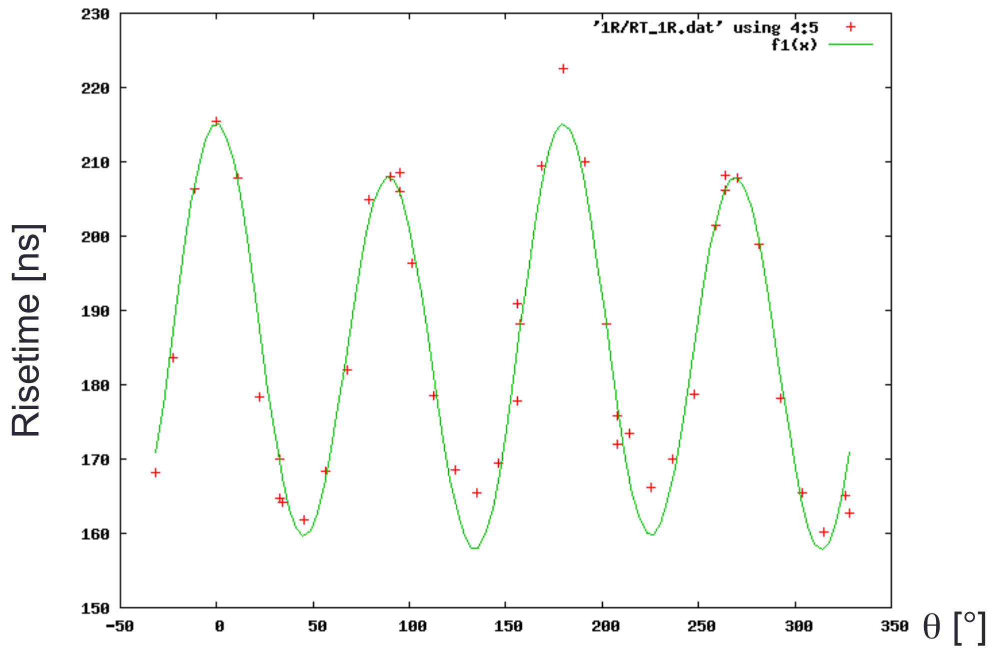
$$v_{100}, v_{111} = \frac{\mu_0 E}{(1 + (\frac{E}{E_0})^{\beta})^{\frac{1}{\beta}}}$$

Measuring the crystal axis



- 400kBq Am source +
- Lead Collimator: ∅ 1.5mm X 1cm
- Front Scan at ∅ 4.7cm: 300 cts/s
- Fitfunction Risetime(θ) =

$$A.[1+R_4\cos(\theta- \theta_4)].[1+R_2\cos(\theta- \theta_2)]$$

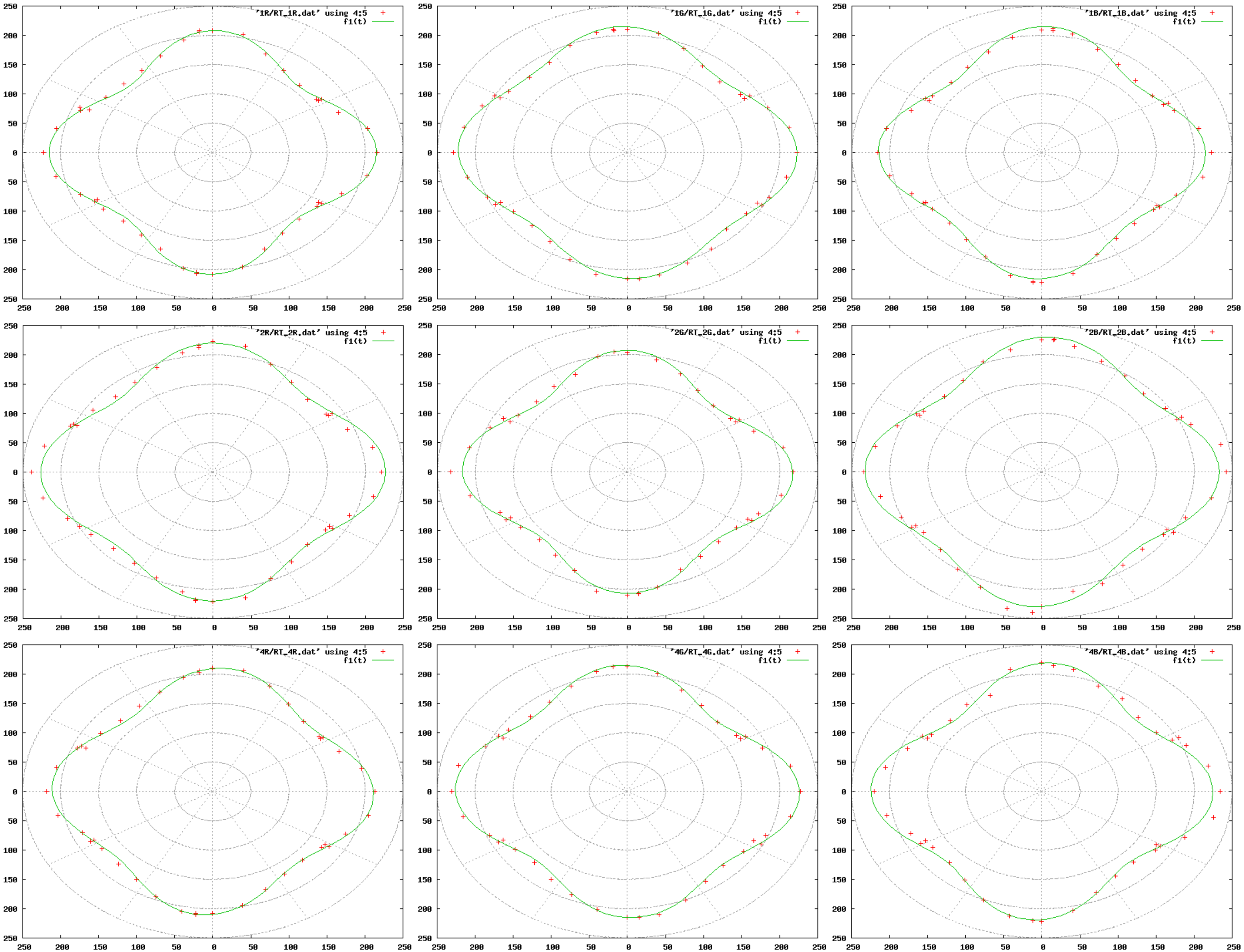


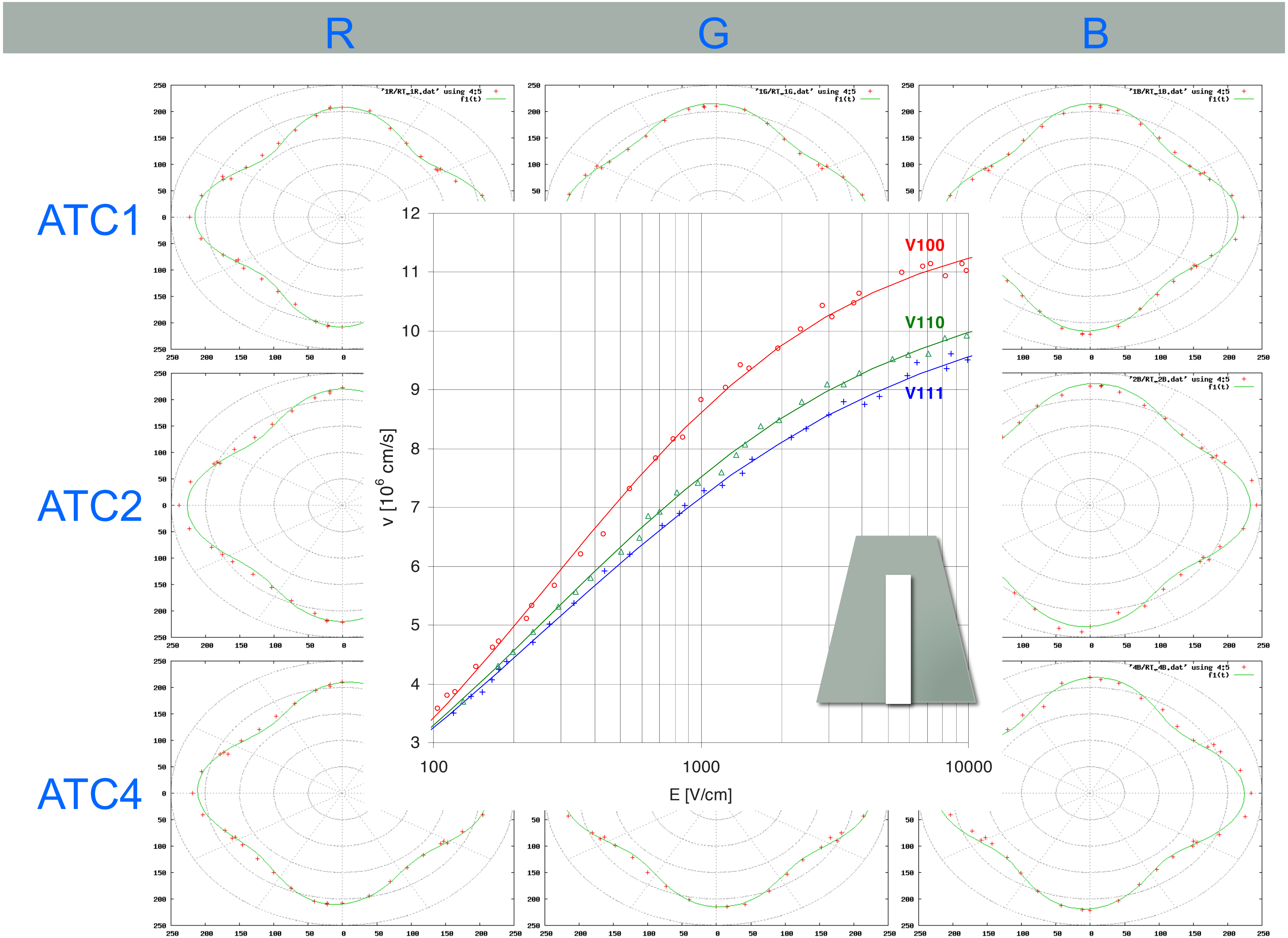
	R	G	B

ATC1

ATC2

ATC4



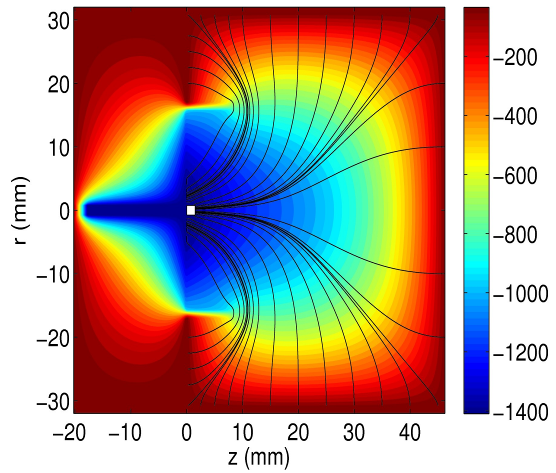


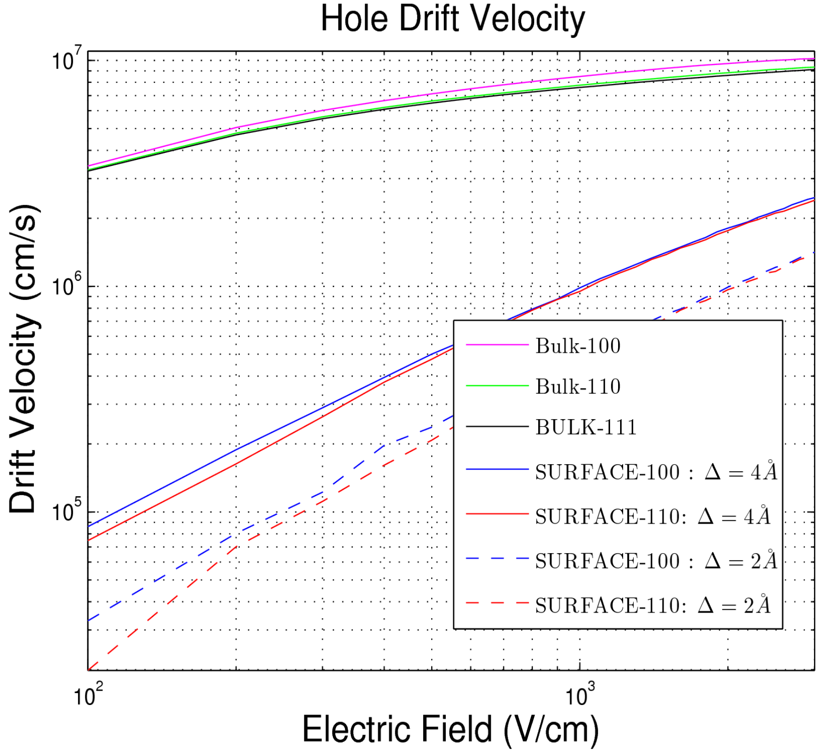
R
G
B
ATC1
ATC2
ATC4
'1R/RT_1R.dat' using 4:5
f1(t)
'1G/RT_1G.dat' using 4:5
f1(t)
'1B/RT_1B.dat' using 4:5
f1(t)
'2B/RT_2B.dat' using 4:5
f1(t)
'4B/RT_4B.dat' using 4:5
f1(t)
V100
V110
V111
v [10^6 cm/s]
E [V/cm]
100
1000
10000

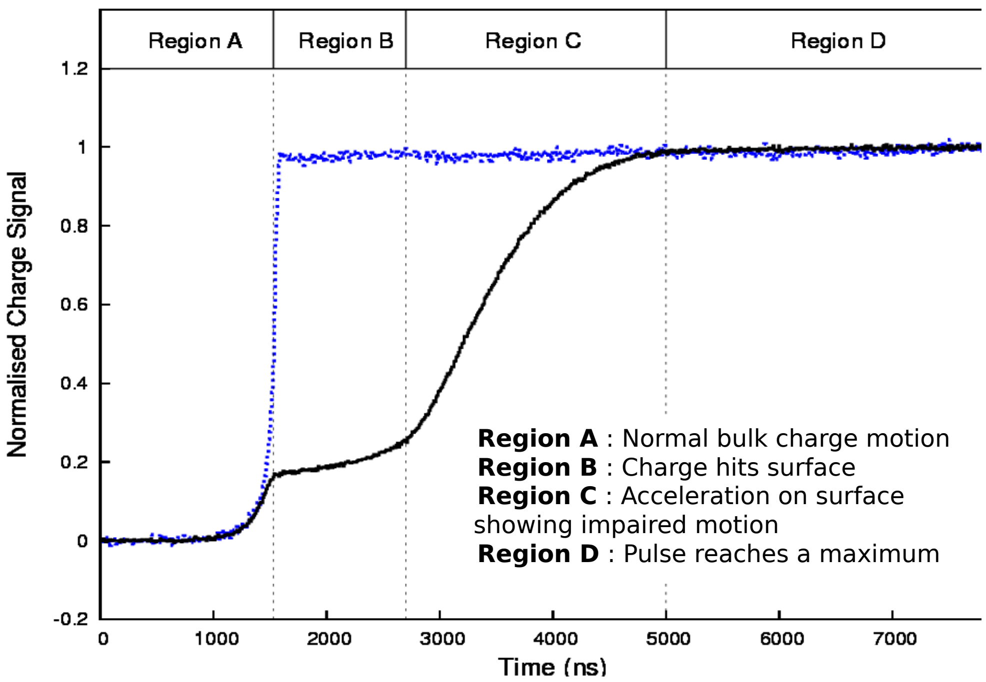
But what at boundaries?

Mullowney et al. NIM A 662 (1) (2012) p.33-44

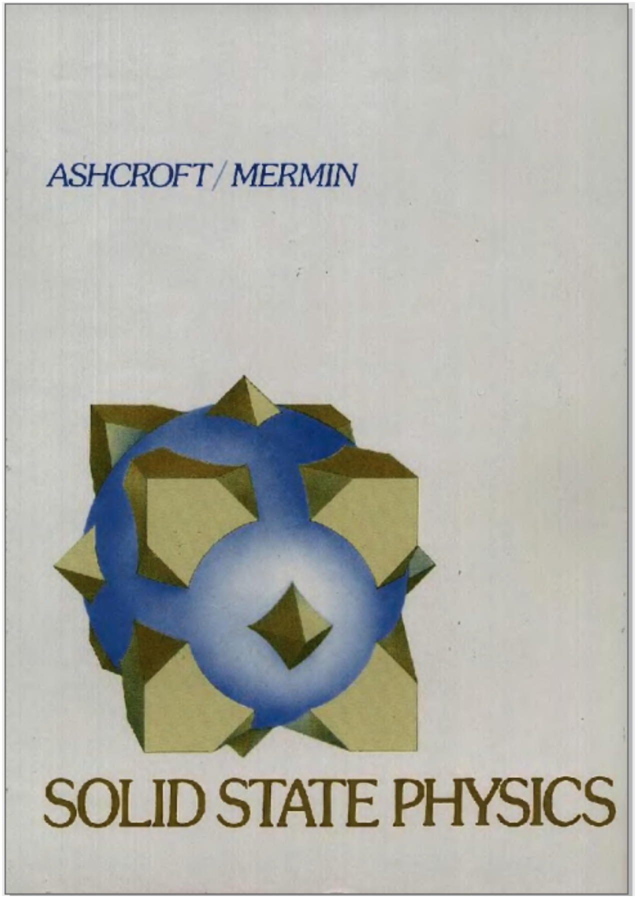
- Particles are trapped to the surface of the interface
- Mobility at interface 2 orders lower

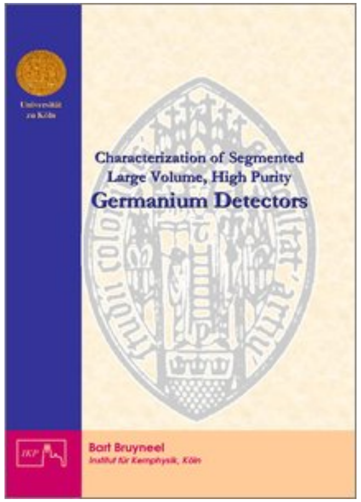


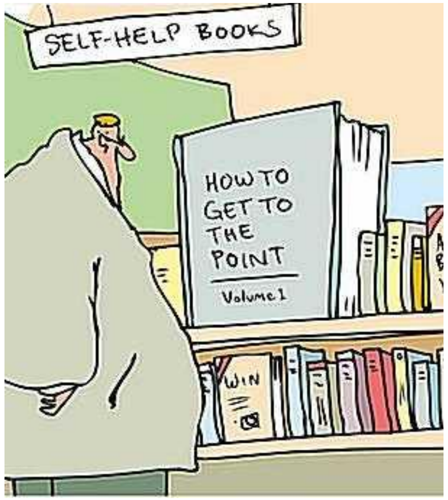




Recommended literature







http://kups.ub.uni-koeln.de/1858/
www.ikp.uni-koeln.de/research/agata/
➔publications
+ references here in

- E. M. Conwell, High field transport in semiconductors, Vol. 9 of Solid State Physics, Academic Press, 1967.