Carrier transport: Evaluation and theory
キャリア輸送: 評価と基礎理論

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Several origins of insulator

- Band insulator

  Finite bandgap

  1. Interference at BZ boundary (metal)
  2. Energy splitting btw bonding – anti-bonding states (covalent)
  3. Energy splitting btw cation and anion levels (ionic)

- Mott insulator

  1. Energy loss by on-site Coulomb U > Energy gain by band formation W
  2. Energy loss by charge transfer from anion (cation) to cation (anion) $\Delta > W$

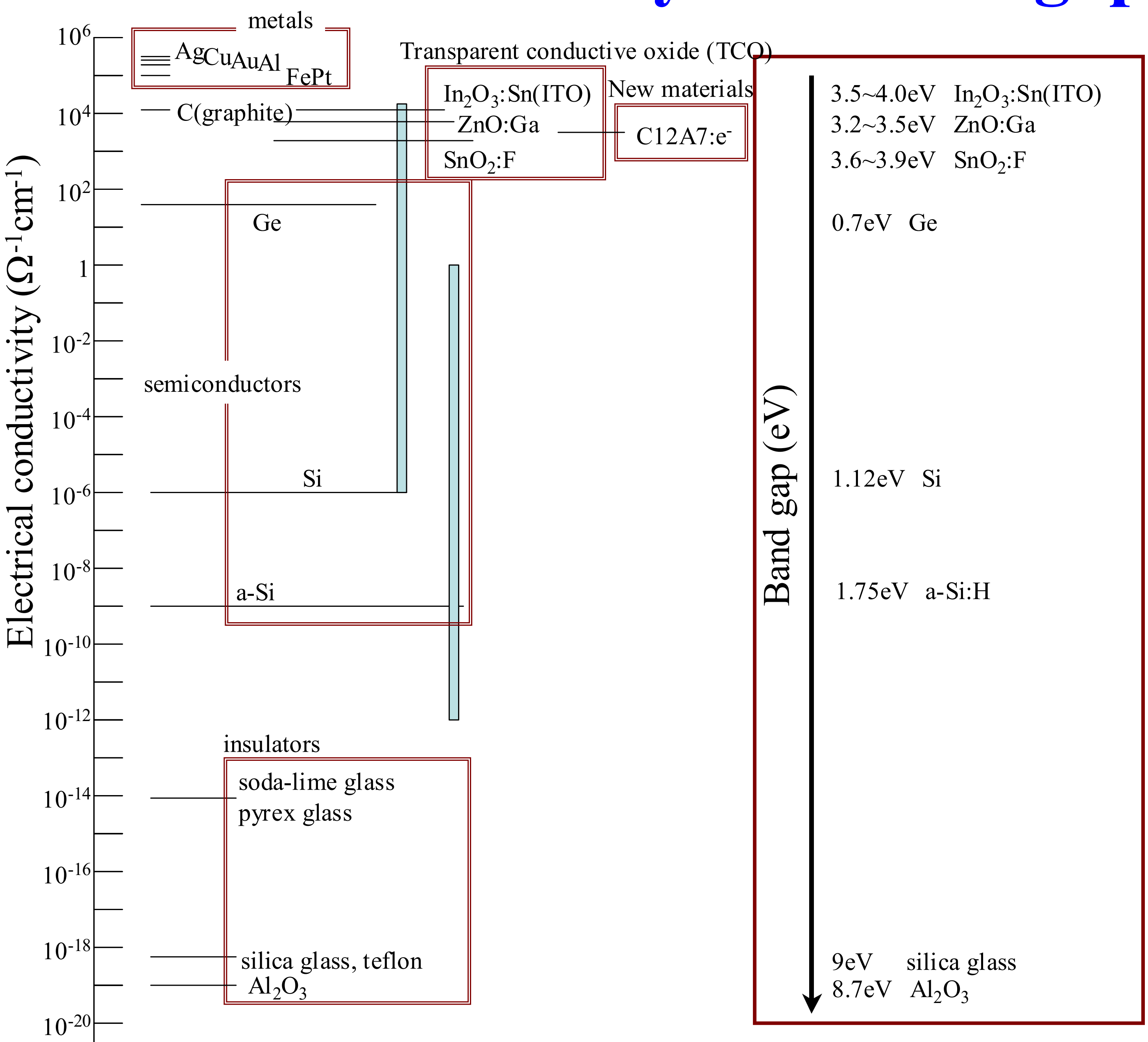
- Localization due to disorder (Anderson localization)

  Localized standing wave formed by interference of scattered wave functions

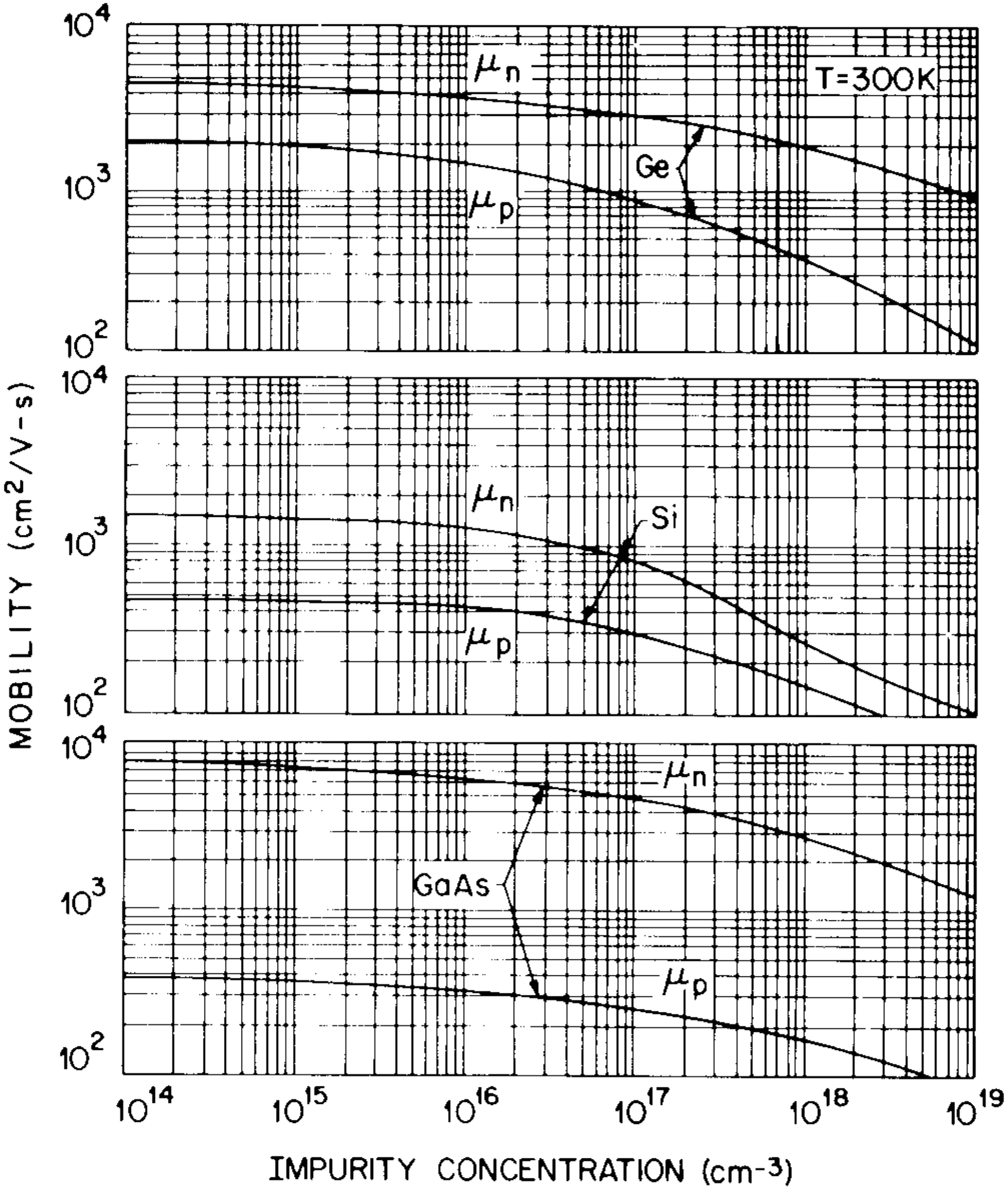
- Topological insulator

  Band gap (zero or finite) is preserved by symmetry of wave function

Electrical conductivity and band gap

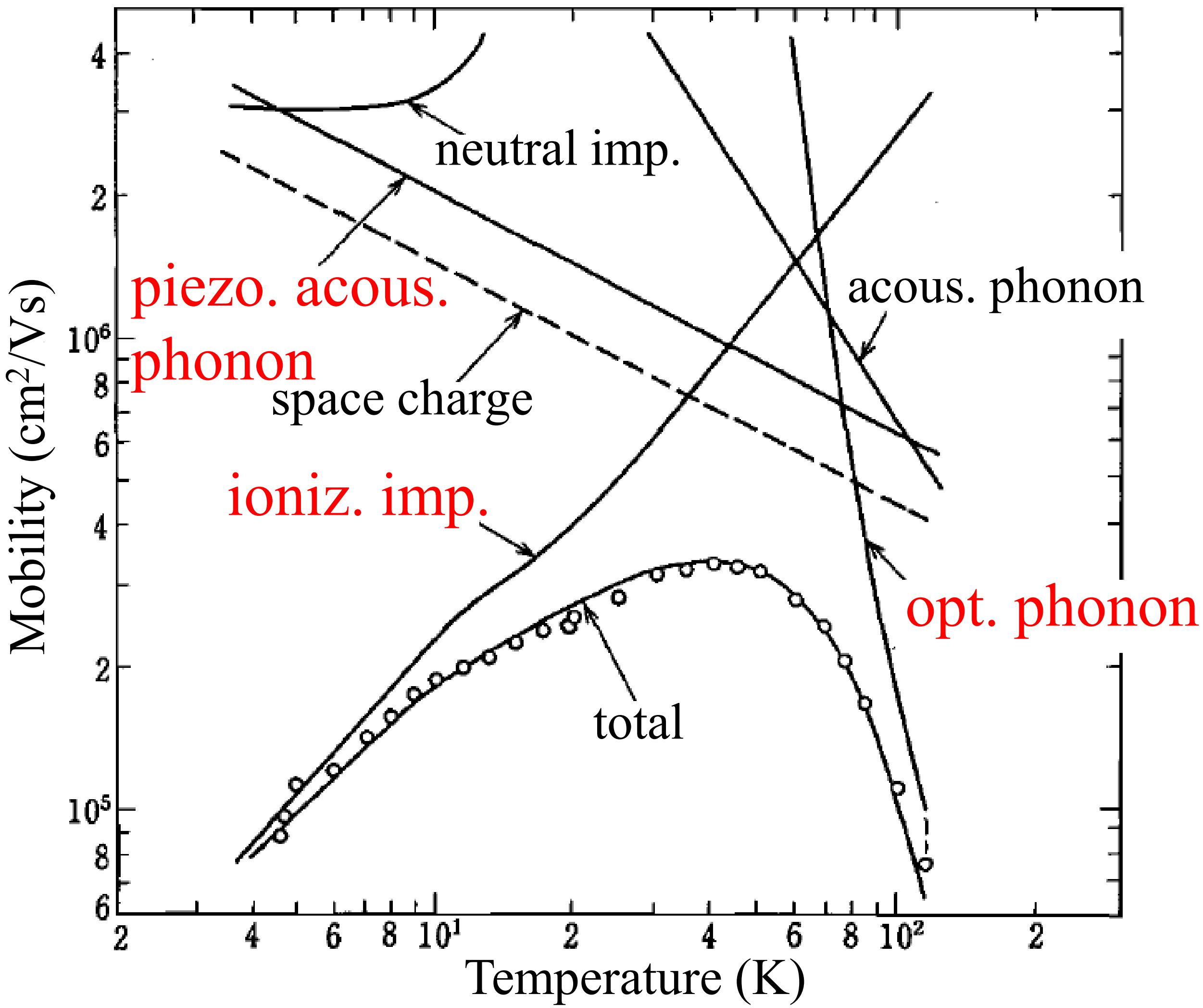


Mobility vs. doping conc.



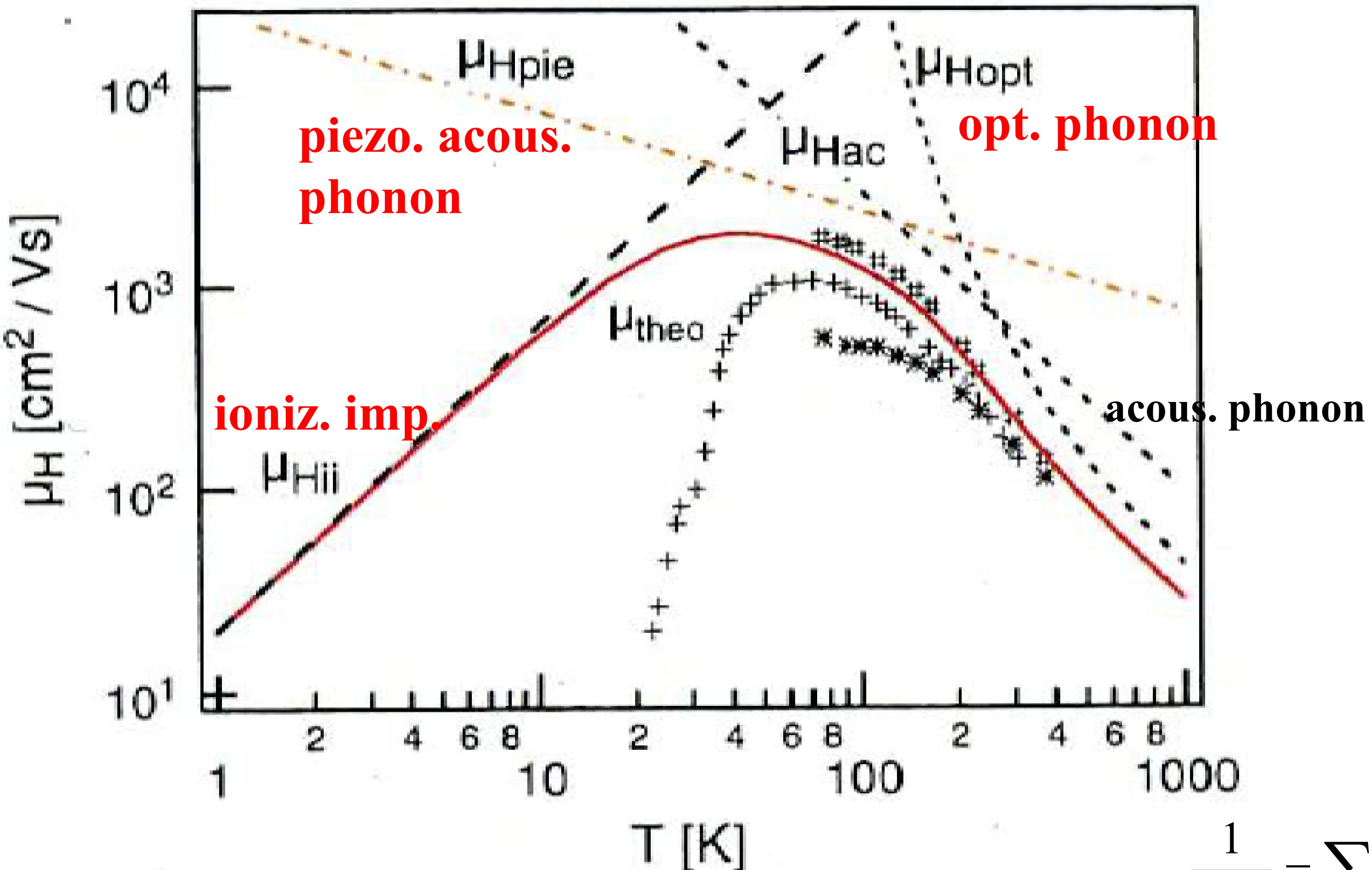
S.M. Sze, Physics of Semiconductor Devices

Mobility in GaAs



$$\frac{1}{\tau(x)} = \sum \frac{1}{\tau_i(x)}$$

Mobility in ZnO



$$\frac{1}{\tau(x)} = \sum \frac{1}{\tau_i(x)}$$

K. Ellmer, Handbook of Transparent Conductors, Fig. 7.13, p.216, Ed. D.S. Ginley (Springer, New York, 2010)

P. Wagner and R. Helbig, J. Phys. Chem. Solids, 35 (1974) 327

Effective masses and relaxation times

	Mobility (cm^2/Vs)	Effective mass (m_e)	τ (10^{-15} s)	Eg (eV)
Si	μ_e=1500 μ_h=500	m_{et}=0.98 m_{el}=0.19 m_{ht}=0.49 m_{hl}=0.16	160 (el)	1.12
In_2O_3:Sn [1)]	μ_e=24~45	m_e=0.3	6.5	3.37
ZnO:Ga [1)]	μ_e=8~25	m_e=0.28~0.33	5.1	3.37
$InGaO_3(ZnO)_5$	**μ_e=16**	**m_e=0.32**	**3.0**	
LaCuOSe:Mg	μ_h=3.4	m_h=1.6	4.2	2.7
C12A7:e^-	μ_e=5.2	m_e=0.82	2.4	7
$Cu_{1.7}Se$	μ_h=5.3	m_h=1.0	3.0	2
a-2CdO·GeO_2	μ_e=12	m_e=0.33	2.3	3.4
a-2CdO·PbO_2	μ_e=10	m_e=0.30	1.7	1.8
a-$InGaO_3(ZnO)_m$ (m=1~4)	**μ_e=13~21**	**m_e=0.34~0.36 (m=1)**	**2.5**	**3.2 – 2.85**
a-$Zn_{0.35}In_{0.35}Sn_{0.3}O_x$	μ_e=10	m_e=0.53	3.9	3.3

[1)] H. Fujiwara and M. Kondo, PRB 71, 075109 (2005)

T dependence of mobility vs scat. mechanism

$$\tau = \tau_0 \varepsilon^{r-1/2} \qquad \mu = \frac{e}{m_e}\langle \tau \rangle = \mu_0 T^s$$

Acoustic photon (Non-degen.)	$\tau = \tau_0 \varepsilon^{-1/2},\ \mu \propto T^{-3/2}$
Acoustic photon (Degenerated)	$\tau = \tau_0 \varepsilon^{-1/2},\ \mu \propto T^{-1}$
Optical photon $T \ll \theta_D$, high-doped	$\tau = \tau_0 \varepsilon^{0},\ \langle \tau \rangle \propto \left[\exp(\hbar\omega_0 / kT) - 1\right]$
Optical photon $T \ll \theta_D$, Low-doped	$\tau = \tau_0 \varepsilon^{0},\ \langle \tau \rangle \propto T^{1/2}$
Ionized impurity (Non-denen.)	$\tau = \tau_0 \varepsilon^{3/2},\quad \mu \propto T^{3/2}$
Ionized impurity (Degenerated)	$\tau = \tau_0 \varepsilon^{3/2},\quad \mu \propto T^{0}$
Neutral impurity	$\tau = \tau_0 \varepsilon^{0},\quad \mu \propto T^{0}$

TABLE 3.2. $\tau = \tau_0 (\varepsilon^*)^{r-1/2}$

Scattering centers, r	τ_0	Notation used
Acoustical vibrations (phonon theory), r = 0	$\frac{9\pi}{4\sqrt{2}} \frac{\hbar^4 \omega^2 M}{C^2 a^8 (m^* kT)^{3/2}}$	ω – velocity of sound; M – atomic mass; C – Bloch constant; a – lattice parameter
Acoustical vibrations (deformation potential theory), r = 0	$\frac{\pi \hbar^4 C_{ll}}{\sqrt{2} E_1^2 (m^* kT)^{3/2}}$	C_{ll} – elastic constant for longitudinal vibrations; $E_1 = \Omega_0 dE_0/d\Omega$; E_0 – energy of allowed band edge; Ω_0 – initial volume of unit cell before deformation
Optical vibrations ($T \ll \theta_D$) in heavily doped crystals, r = 1/2	$\frac{a^3 M}{2\pi\sqrt{2m^*}} \frac{(\hbar\omega_0)^{3/2}}{(\gamma Z e^2)^2} \times \left[\exp\left(\frac{\hbar\omega_0}{kT}\right) - 1\right](1 - f_0)$	ω_0 – limiting frequency of longitudinal optical vibrations; Ze – ion charge; γ – factor representing the polarizability of ions; f – Fermi function; θ_D – Debye temperature
Optical vibrations ($T \ll \theta_D$) in lightly	$\frac{a^3 M}{2\pi\sqrt{2m^*}} \frac{(\hbar\omega_0)^{3/2}}{(\gamma Z e^2)^2} \times$	

TABLE III. Approximate ϵ and T dependencies for electron-scattering mechanisms.

Scattering mechanism	Energy dependence of τ	τ	Temperature dependence of μ^{nondegen}	μ^{degen}
Intravalley acoustic phonons	$\epsilon^{-1/2}$	T^{-1}	$T^{-3/2}$	T^{-1}
Intervalley optical phonons	$\epsilon^{-1/2}$	T^{-1}	$T^{-3/2}$	T^{-1}
Ionized impurities	$\epsilon^{3/2}$	T^{0}	$T^{3/2}$	T^{0}
Alloy disorder	$\epsilon^{-1/2}$	T^{0}	$T^{-1/2}$	T^{0}
Neutral impurities	ϵ^{0}	T^{0}	T^{0}	T^{0}

Heavily doped semiconductor, P.86

A model for the high-temperature transport properties of heavily doped n-type silicon-germanium alloys, JAP 69 (1991) 331 Fig. 3

Simple model of carrier transport

簡単なモデル解析

What is carrier mobility?

$$\sigma = en\mu$$

Definition in solid-state physics

Drift mobility $\mu_d = \frac{v_d}{E} = \frac{e}{m_e}\tau$

Motion of dynamic for an e^- $F = m_e\left(\frac{d}{dt}v - \frac{1}{\tau}v\right) = qE$

m_e: Effective mass

τ : Momentum relaxation time (scattering time)

Average time for an electron to loose its momentum by scattering

Steady-state velocity $v = \frac{e}{m_e}\tau E$

Drift velocity v_d: Velocity driven by electric field

⇔ thermal velocity, Fermi velocity, diffusion velocity etc

Band conduction mobility limit

$$v_{th} = \sqrt{2m_e^* k_B T} = 2\times10^5 \text{ m/s}$$

$l_{\text{th}} = v_{\text{th}}\tau >>$ inter atomic distance

In-In distance in a-IGZO: 3.1 Å

=> $\tau >> 1.5$ fs

$$\mu = \frac{e\tau}{m_e^*}$$

$m_{\text{e}}^* = 0.35\, m_{\text{e}}$ →

$\mu >> 8$ cm^2/Vs for band conduction

But: Hall mobility ~ 0.2 cm^2/Vs in IGZO

$l_{\text{th}} = 0.1$ Å ???

Several kinds of current generation / annihilation

$$\frac{d(n+\Delta n)}{dt} = \frac{1}{e}\nabla \mathbf{J}_n + G_n - U_n \qquad \mathbf{J} = eD\nabla n + en\frac{e\langle\tau\rangle}{m_e^*}\mathbf{E}$$

$$\frac{d\Delta n(x)}{dt} = D_n \frac{\partial^2 \Delta n(x)}{\partial x^2} + \mu_n E(x)\frac{\partial \Delta n(x)}{\partial x} + G_n(x) - \frac{\Delta n(x)}{\tau_n}$$

$$\frac{d\Delta p(x)}{dt} = D_p \frac{\partial^2 \Delta p(x)}{\partial x^2} + \mu_p E(x)\frac{\partial \Delta p(x)}{\partial x} + G_p(x) - \frac{\Delta p(x)}{\tau_p}$$

Time variation Diffusion Drift Generation Recombination

Fermi level E_F is defined only under equribirum
Mimic for non-equilibrium states: Quasi Fermi vlevel

$$n = n_0 + \Delta n = N_\mathrm{c}\exp\left(-\frac{E_\mathrm{c} - E_{\mathrm{F}n}}{k_\mathrm{B}T}\right) \qquad p = p_0 + \Delta p = N_\mathrm{v}\exp\left(-\frac{E_{\mathrm{F}p} - E_\mathrm{v}}{k_\mathrm{B}T}\right)$$

Hall effect: Simple explanation

Charge *q* (electron: -*e*, hole: +*e*)

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

$$m^*\left(\frac{d}{dt} + \frac{1}{\tau}\right)\mathbf{v} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

$$m^*\left(\frac{d}{dt} + \frac{1}{\tau}\right)v_x = q(E + Bv_y)$$

$$m^*\left(\frac{d}{dt} + \frac{1}{\tau}\right)v_y = q(-Bv_x) \qquad m^*\left(\frac{d}{dt} + \frac{1}{\tau}\right)v_z = 0$$

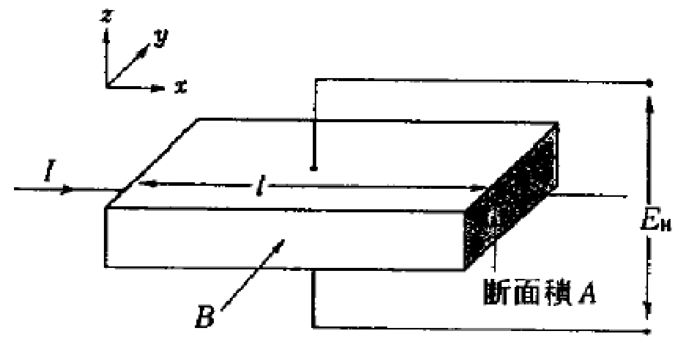


図 3·24 Hall 効果の実験

$$v_x = -\frac{e\tau}{m^*}E - \omega_c \tau v_y$$

$$v_y = \omega_c \tau v_x \qquad v_z = 0 \qquad \omega_c = qB/m^*c$$

$$m^*\left(\frac{d}{dt} + \frac{1}{\tau}\right)v_y = q(E_{Hall} - Bv_x)$$

$$E_{Hall} = \frac{B}{c}v_x = \frac{qB\tau}{m^*c}E \qquad j_x = \frac{nq^2\tau}{m^*}E_x$$

$$R_H = \frac{E_{Hall}}{j_x B} = \frac{1}{nq}$$

Carrier polarity (sign of R_H), density n_{Hall}, mobility μ_{Hall}

Hall effect

太田英二、坂田亮著、半導体の電子物性光学、培風館 (2005)

–e: Electron charge, Under E_x and B_z

Motion of dynamics $$m_e^*\left(\frac{d\boldsymbol{v_i}}{dt}+\frac{\boldsymbol{v_i}}{\tau}\right)=-e(\boldsymbol{E}+\boldsymbol{v_i}\times\boldsymbol{B})$$

Average velocity $\langle\boldsymbol{v}\rangle=\sum\boldsymbol{v_i}/n$

$$m_e^*\left(\frac{d\langle\boldsymbol{v}\rangle}{dt}+\frac{\langle\boldsymbol{v}\rangle}{\tau}\right)=-e(\boldsymbol{E}+\langle\boldsymbol{v}\rangle\times\boldsymbol{B})$$

$$m_e^*\langle\boldsymbol{v}\rangle_x=-e\tau\left(E_x+\langle\boldsymbol{v}\rangle_y B_z\right)$$

$$m_e^*\langle\boldsymbol{v}\rangle_y=-e\tau\left(E_y-\langle\boldsymbol{v}\rangle_x B_z\right)$$

$$m_e^*\langle\boldsymbol{v}\rangle_z=-e\tau E_z$$

$$\langle\boldsymbol{v}\rangle_x=-\frac{e\tau}{m_e^*}\frac{E_x+\frac{e\tau}{m_e^*}B_zE_y}{1+\left(\frac{e\tau}{m_e^*}\right)^2{B_z}^2}$$

$$\langle\boldsymbol{v}\rangle_y=-\frac{e\tau}{m_e^*}\frac{E_y-\frac{e\tau}{m_e^*}B_zE_x}{1+\left(\frac{e\tau}{m_e^*}\right)^2{B_z}^2}$$

$$\langle\boldsymbol{v}\rangle_x=-\frac{e\tau}{m_e^*}E_z$$

Hall effect

太田英二、坂田亮著、半導体の電子物性光学、培風館 (2005)

Current $$\boldsymbol{J} = -e\langle \boldsymbol{v} \rangle = \frac{e^2 n\tau}{m_e^*}\begin{pmatrix} \dfrac{1}{1+\left(\frac{e\tau}{m_e^*}\right)^2 {B_z}^2} & \dfrac{\left(\frac{e\tau}{m_e^*}\right)B_z}{1+\left(\frac{e\tau}{m_e^*}\right)^2 {B_z}^2} & 0 \\ -\dfrac{\left(\frac{e\tau}{m_e^*}\right)B_z}{1+\left(\frac{e\tau}{m_e^*}\right)^2 {B_z}^2} & \dfrac{1}{1+\left(\frac{e\tau}{m_e^*}\right)^2 {B_z}^2} & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}$$

$$= \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ \sigma_{yx} & \sigma_{yy} & 0 \\ 0 & & \sigma_{zz} \end{pmatrix}\begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}$$

$$= \sigma_{xx}\left[\boldsymbol{E} + \left(\frac{e\tau}{m_e^*}\right)^2 \boldsymbol{B}(\boldsymbol{E}\cdot\boldsymbol{B}) + \frac{e\tau}{m_e^*}(\boldsymbol{E}\times\boldsymbol{B})\right]$$

$\omega_c = \left(\frac{e}{m_e^*}\right)B_z$: cyclotron frequency

Hall effect

太田英二、坂田亮著、半導体の電子物性光学、培風館 (2005)

Upon $J_y = 0$

$$\frac{e^2 n\tau}{m_e^*}\begin{pmatrix} \dfrac{1}{1+\left(\dfrac{e\tau}{m_e^*}\right)^2 {B_z}^2} & \dfrac{\left(\dfrac{e\tau}{m_e^*}\right)B_z}{1+\left(\dfrac{e\tau}{m_e^*}\right)^2 {B_z}^2} \\ -\dfrac{\left(\dfrac{e\tau}{m_e^*}\right)B_z}{1+\left(\dfrac{e\tau}{m_e^*}\right)^2 {B_z}^2} & \dfrac{1}{1+\left(\dfrac{e\tau}{m_e^*}\right)^2 {B_z}^2} \end{pmatrix}\begin{pmatrix} E_x \\ E_y \end{pmatrix} = \begin{pmatrix} J_x \\ J_y \end{pmatrix}$$

$$E_x = \frac{J_x \sigma_{xx}}{\sigma_{xx}\sigma_{yy} - \sigma_{yx}\sigma_{yx}} = \frac{1}{\sigma_0} J_x$$

$$E_y = -\frac{J_x \sigma_{yz}}{\sigma_{xx}\sigma_{yy} - \sigma_{yx}\sigma_{yx}} = -\frac{1}{en} B_z J_x = R_H B_z J_x$$

$$\boldsymbol{R_H = -\frac{E_y}{B_z J_x}} = -\frac{V_H}{W}\frac{Wd}{I_x}\frac{1}{B_z} \boldsymbol{= -\frac{V_H}{I_x}\frac{d}{B_z}}$$ **(for electron)**

Hall effect: Two-carrier model

太田英二、坂田亮著、半導体の電子物性光学、培風館 (2005)

When electrons and holes coexist

$$\boldsymbol{J_e} = \sigma_e \boldsymbol{E} - \sigma_e \mu_e \boldsymbol{E} \times \boldsymbol{B}$$
$$\boldsymbol{J_h} = \sigma_h \boldsymbol{E} + \sigma_h \mu_h \boldsymbol{E} \times \boldsymbol{B}$$
$$\boldsymbol{J} = \boldsymbol{J_e} + \boldsymbol{J_e} = (\sigma_e + \sigma_h)E + (-\sigma_e \mu_e + \sigma_h \mu_h)\boldsymbol{E} \times \boldsymbol{B}$$

$$R_H = \frac{n_h {\mu_h}^2 - n_e {\mu_e}^2}{e(n_h \mu_h + n_e \mu_e)^2}$$

(i) Only holes: $\boldsymbol{n_e = 0}$ => $\boldsymbol{R_H = \frac{\mu_h}{e n_h}}$

(ii) Same mobility: $\boldsymbol{\mu_h = \mu_e = \mu}$ => $\boldsymbol{R_H = \frac{n_h - n_e}{e(n_h + n_e)^2}}$

(iii) Nearly intrinsic: $\boldsymbol{n_h \sim n_e \sim n_i}$ => $\boldsymbol{R_H = \frac{1 - \mu_e/\mu_h}{e n_i (1 + \mu_e/\mu_h)}}$

R_H for multi band / mixed carriers

Multi band / Multi layers

$$R_H = \gamma \sum \frac{\mathrm{sgn}_i \, n_i \mu_i^2}{q\left(\sum n_i \mu_i\right)^2} \qquad \sigma = q \sum n_i \mu_i$$

Electron – hole mixed conduction

$$R_H = \gamma \sum \frac{p\mu_p^2 - n\mu_n^2}{q\left(n\mu_n + p\mu_p\right)^2} \qquad \sigma = q \sum n_i \mu_i$$

Magnetoresistance: Drude model

太田英二、坂田亮著、半導体の電子物性光学、培風館 (2005)

Current $\boldsymbol{J} = -e\langle \boldsymbol{v} \rangle = \frac{e^2 n\tau}{m_e^*} \begin{pmatrix} \frac{1}{1+\left(\frac{e\tau}{m_e^*}\right)^2 {B_z}^2} & \frac{\left(\frac{e\tau}{m_e^*}\right)B_z}{1+\left(\frac{e\tau}{m_e^*}\right)^2 {B_z}^2} & 0 \\ -\frac{\left(\frac{e\tau}{m_e^*}\right)B_z}{1+\left(\frac{e\tau}{m_e^*}\right)^2 {B_z}^2} & \frac{1}{1+\left(\frac{e\tau}{m_e^*}\right)^2 {B_z}^2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}$

Two carrier model

$$\boldsymbol{J} = \boldsymbol{J_e} + \boldsymbol{J_e} = (\sigma_e + \sigma_h)E + (-\sigma_e\mu_e + \sigma_h\mu_h)\boldsymbol{E} \times \boldsymbol{B}$$

$$\rho_{xx}(B) = \mathrm{Re}(\rho) = \frac{1}{e}\frac{(n_h\mu_h + n_e\mu_e) + (n_h\mu_e + n_e\mu_h)\mu_h\mu_e B^2}{(n_h\mu_h + n_e\mu_e)^2 + (n_h - n_e)^2\mu_h^2\mu_e^2 B^2},$$

$$\rho_{yx}(B) = -\mathrm{Im}(\rho) = \frac{B}{e}\frac{(n_h\mu_h^2 - n_e\mu_e^2) + (n_h - n_e)\mu_h^2\mu_e^2 B^2}{(n_h\mu_h + n_e\mu_e)^2 + (n_h - n_e)^2\mu_h^2\mu_e^2 B^2}.$$

Two carrier model of MR

MR-TwoCarriermodel.py (to be uploaded for Lab only web)

e.g. in APL 107, 182411 (2015)

$$\rho_{xx}(B) = \mathrm{Re}(\rho) = \frac{1}{e}\frac{(n_h\mu_h + n_e\mu_e) + (n_h\mu_e + n_e\mu_h)\mu_h\mu_e B^2}{(n_h\mu_h + n_e\mu_e)^2 + (n_h - n_e)^2\mu_h^2\mu_e^2 B^2},$$

$$\rho_{yx}(B) = -\mathrm{Im}(\rho) = \frac{B}{e}\frac{(n_h\mu_h^2 - n_e\mu_e^2) + (n_h - n_e)\mu_h^2\mu_e^2 B^2}{(n_h\mu_h + n_e\mu_e)^2 + (n_h - n_e)^2\mu_h^2\mu_e^2 B^2}.$$

of parameters must be larger than # of constraints,

of parameters: four n_h, μ_h, n_e, μ_e

# of constraints: three

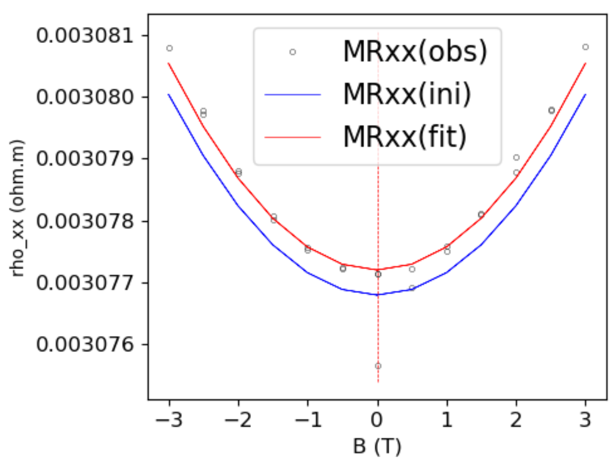
For parabolic $\rho_{xx}(B)$: $a_{xx}^0 = \rho_{xx}(0)$, and a_{xx}^2

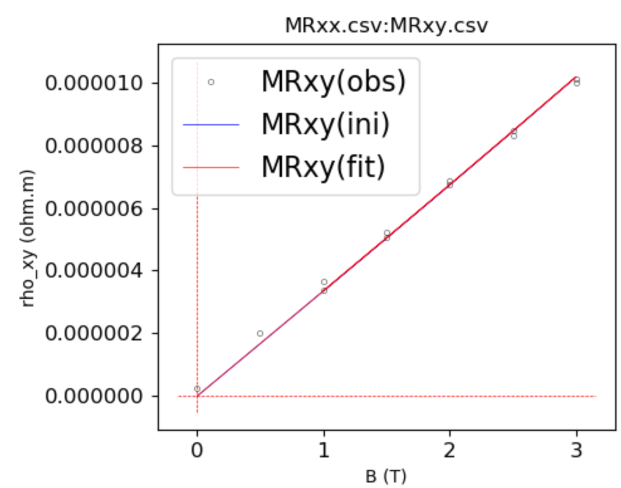
For linear $\rho_{xy}(B)$: a_{xy}^1 only

At least two parameter sets give similar residuals S^2

$n_h = 2.09\text{x}10^{23}$ m^{-3}
$\mu_h = 0.074$ m^2/Vs
$n_e = 2.72\text{x}1022$ m^{-3}
$\mu_e = 0.018$ m^2/Vs
$S^2 = 3.2\text{x}10^{-14}$

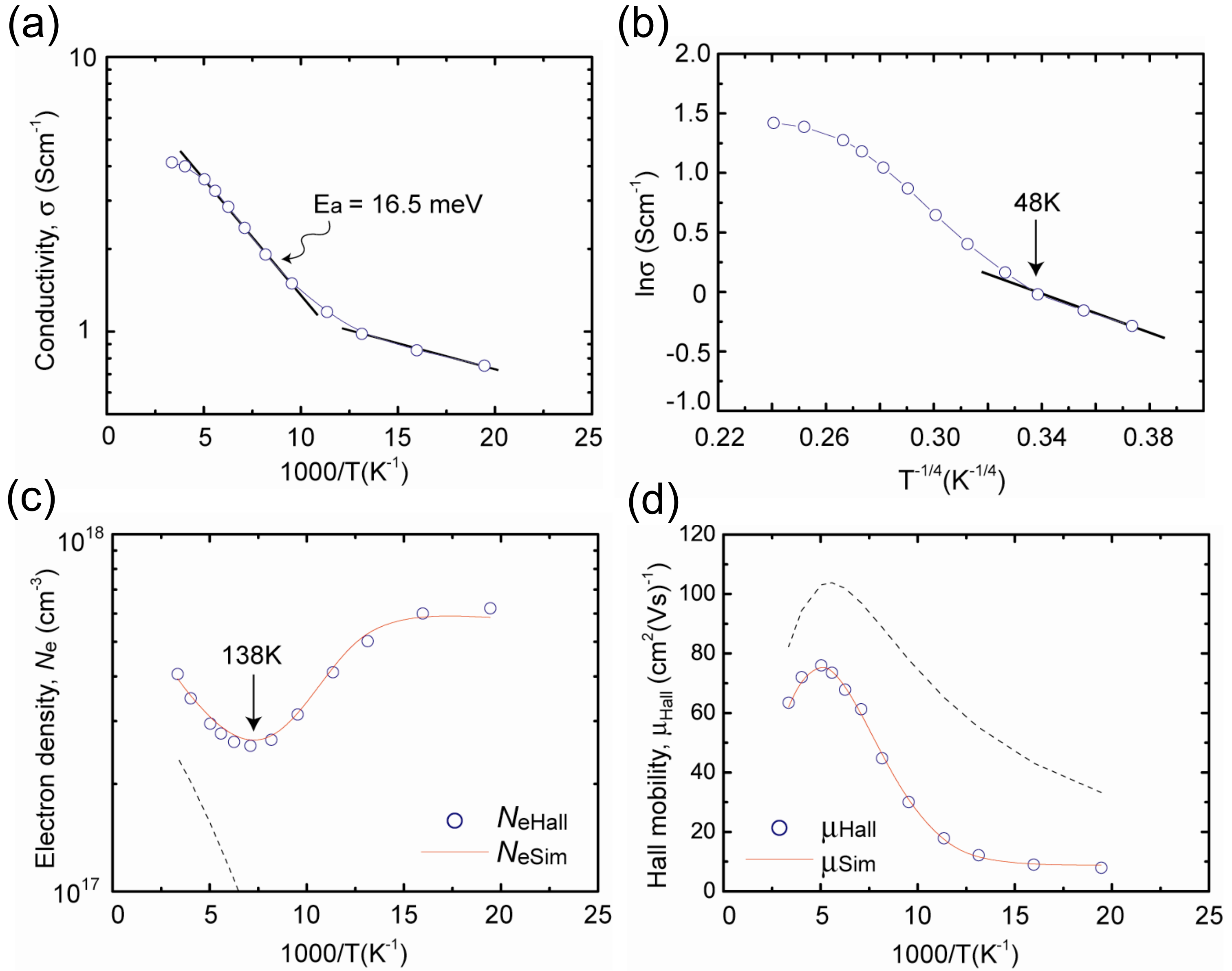
$n_h = 9.23\text{x}10^{22}$ m^{-3}
$\mu_h = \mu_e = 0.012$ m^2/Vs
$n_e = 7.68\text{x}1022$ m^{-3}
$S^2 = 3.0\text{x}10^{-14}$





Apparent n_{Hall} anomaly in ZnO/ScAlMgO$_4$

Katase et al., Cryst. Growth&Des. ***10****, 1084 (2010)*



Non-equilibrium statistics dynamics

非平衡統計力学

Calculation procedure under equilibrium

1. Determine parameters e.g. m_e^*
2. Calculate constants e.g. N_c, D_{c0}
3. Build density-of-states function D(E)
4. Calculate the number of electrons in the energy range considered (usually considered at 0 K for neutral state): Charge neutrality condition
5. Draw band structure – position diagram by assuming constant E_F to determine functions of conduction band minimum (CBM) and valence band maximum (VBM), $E_{CBM}(x)$, $E_{VBM}(x)$
6. Calculate extra charge distributions

   $$\rho_e(x) = N_c \exp(-(E_{CBM}(x)-E_F)/k_BT)$$
   $$\rho_h(x) = N_v \exp(-(E_F-E_{VBM}(x))/k_BT)$$

   from $E_{CBM}(x)$ and $E_{VBM}(x)$
7. Solve 5-6 self-consistently so as to satisfy Possison equation

   $$d^2E_{CBM}(x)/dx^2 = e(-\rho_e(x)+\rho_h(x)+N_D^+(x)-N_A^-(x))\ /\varepsilon$$

For non-equilibrium state

Equilibrium: No time variation for macroscopic quantities
Closed system

Steady state: No time variation for macroscopic quantities
Exchange of energy / particles etc btw external system

Steady states, but not equilibrium

- Electron flow btw external system
- Bias, temperature distribution etc
- E_F is not uniform over the system

- Boltzmann transport theory
- Current continuity equation

Non-equilibrium statistical physics

Under equilibrium

Fermi-Dirac distribution function $$f_0(E) = \frac{1}{1 + \exp[(E - E_{F0})/k_B T]}$$

Density-of-states function $$D(E)$$

Distribution of electrons actually occupying *D*(*E*) $$n_0(E) = f_0(E)D(E)$$

Non-equilibrium state: Main approach is to find distribution function $f(E, \mathbf{r}, \mathbf{k}, t)$

$$f(E, \mathbf{r}, \mathbf{k}, t) = f_0(E) + f_1(E)$$

Boltzmann's transport equation

Boltzmann equation

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t}\right)_{r,k} + \frac{dr}{dt}\nabla_r f + \frac{dk}{dt}\nabla_k f$$

$$\mathbf{F} = \hbar\frac{d\mathbf{k}}{dt} \qquad \mathbf{v_k} = \frac{d\mathbf{r}}{dt}$$

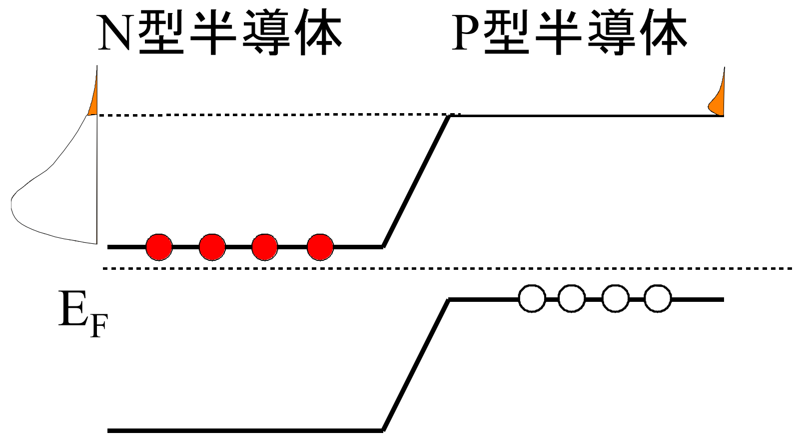
$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t}\right)_{\mathbf{r},\mathbf{k}} + \mathbf{v_k}\nabla_{\mathbf{r}} f + \frac{\mathbf{F}}{\hbar}\nabla_{\mathbf{k}} f$$

Diffusion term **Drift term**

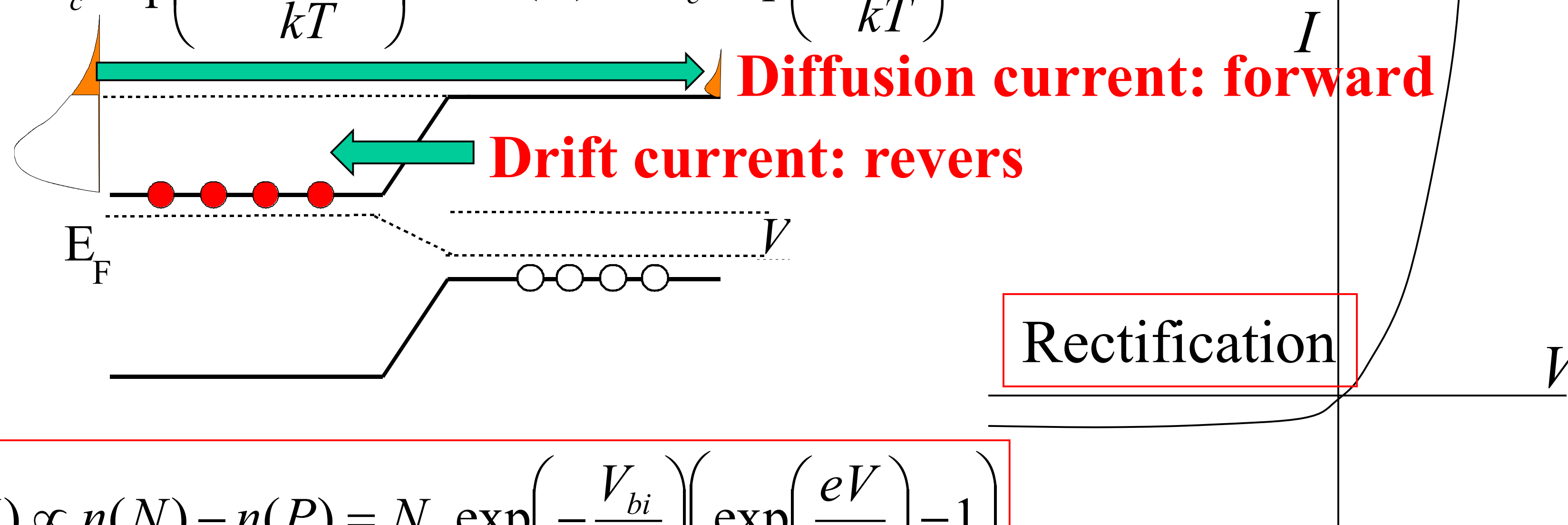
Under electric field *E*

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t}\right)_{r,k} + v_k\nabla_r f - e\frac{E}{\hbar}\nabla_k f$$

P/N diode: Diffusion-current device



$$n(N) = N_c \exp\left(-\frac{V_{bi} - V}{kT}\right) \qquad n(P) = N_c \exp\left(-\frac{V_{bi}}{kT}\right)$$



$$J(V) \propto n(N) - n(P) = N_c \exp\left(-\frac{V_{bi}}{kT}\right)\left(\exp\left(\frac{eV}{kT}\right) - 1\right)$$

Thermoelectric device: Diffusion current

Different T for a material T_H, T_L
Electrons are re-distributed so as to reach uniform E_F

Metal: Electron density independent of T

Kinetic energy $\sim \boldsymbol{E_F^0} + \frac{1}{2}\boldsymbol{m}\boldsymbol{v_{th}}^2$

$$\langle \boldsymbol{v_x} \rangle \sim \frac{1}{2}\boldsymbol{kT}$$

Difference in thermal velocity causes diffusion from T_H to T_L

Semiconductor: Electron density $\boldsymbol{N_C}\mathbf{exp}\left(-\frac{\boldsymbol{E_C}-\boldsymbol{E_F}}{\boldsymbol{kT}}\right)$

Difference in electron density causes diffusion from T_H to T_L

Relaxation time approx. for scattering term

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t}\right)_{\mathbf{r},\mathbf{k}} \qquad + \mathbf{v_k}\nabla_\mathbf{r} f \qquad + \frac{\mathbf{F}}{\hbar}\nabla_\mathbf{k} f$$

$$\frac{df}{dt} = -\frac{f - f_0}{\tau}$$

$$\frac{df}{d\mathbf{k}} = \frac{\partial f}{\partial E}\frac{\partial E}{\partial \mathbf{k}} = \hbar \mathbf{v_k}\frac{\partial f}{\partial E} \qquad \mathbf{v_k} = \frac{1}{\hbar}\frac{\partial E}{\partial \mathbf{k}}$$

Boltzmann-Bloch equation (for steady state)

$$-\frac{f - f_0}{\tau} = \mathbf{v_k}\nabla_\mathbf{r} f + \frac{\mathbf{F}}{\hbar}\nabla_\mathbf{k} f$$

$$-\frac{f - f_0}{\tau} = \left(\frac{\partial f}{\partial t}\right)_{\mathbf{r},\mathbf{k}} + \mathbf{v_k}\nabla_\mathbf{r} f + \mathbf{v_k}\mathbf{F}\frac{\partial f}{\partial E}$$

$$f \sim f_0 - \tau\left(\frac{\partial f_0}{\partial t}\right)_{r,k} - \tau v_k \nabla_r f_0 - \tau v_k F \frac{\partial f_0}{\partial E}$$

Equations to solve electron transport

Charge neutrality condition

$$\int_{E_C}^{\infty} D_C(E) f(E) dE + N_A{}^{-} = \int_{E_C}^{\infty} D_V(E)[1 - f(E)] dE + N_D{}^{+}$$

Poisson equation

$$\nabla^2 \varphi(x) = \frac{\rho(x)}{\varepsilon}$$

$$\rho(x) = -e[n(x) + N_A{}^{-}] + e\left[p(x) + N_D{}^{+}\right]$$

$$n(x) = \int_{E_C}^{\infty} D_C(E) f(E) dE \qquad p(x) = \int_{-\infty}^{E_V} D_V(E)[1 - f(E)] dE$$

Transport equation

$$f \sim f_0 - \tau \left(\frac{\partial f_0}{\partial t}\right)_{\mathbf{r},\mathbf{k}} - \tau \mathbf{v}_{\mathbf{k}} \nabla_{\mathbf{r}} f_0 - \tau \mathbf{v}_{\mathbf{k}} \mathbf{F} \frac{\partial f_0}{\partial E}$$

Band structure and *E*

$\mathbf{E}_e = -\nabla_{\mathbf{r}} E_C$ **Effective mass approx.** $E - E_C = \dfrac{\hbar^2}{2m_e^*} \mathbf{k}^2$

Current density vs E

$$f \sim f_0 - \tau\left(\frac{\partial f_0}{\partial t}\right)_{t,\mathbf{r},\mathbf{k}} - \tau\mathbf{v_k}\nabla_\mathbf{r} f_0 - \tau\mathbf{v_k}\mathbf{F}\frac{\partial f_0}{\partial E} = f_0 + e\tau\mathbf{v_k}\mathbf{E}\frac{\partial f_0}{\partial E}$$

$$\begin{aligned}\mathbf{J} = -e\int \mathbf{v_k}\, dk_x dk_y dk_z \\ = -e\int \mathbf{v_k} D(E) f(E)\, dE \\ = -e\int \mathbf{v_k} D(E)\left[f_0 + e\tau\mathbf{v_k}\mathbf{E}\frac{\partial f_0}{\partial E}\right] dE \\ = -e\int \mathbf{v_k} D(E)\left[e\tau\mathbf{v_k}\mathbf{E}\frac{\partial f_0}{\partial E}\right] dE\end{aligned}$$

$$\boldsymbol{J_x = -e^2\int v_x{}^2\tau(E)D(E)\frac{\partial f_0}{\partial E}dE\cdot E_x = -\frac{e^2}{k_B T}\int v_x{}^2\tau(E)D(E)f_0(1-f_0)dE\cdot E_x}$$

$$\frac{\partial f_0}{\partial E} = \frac{1}{k_B T} f_0(1-f_0)$$

Current density vs E

$$f \sim f_0 - \tau \left(\frac{\partial f_0}{\partial t}\right)_{t,\mathbf{r},\mathbf{k}} - \tau \mathbf{v_k} \nabla_{\mathbf{r}} f_0 - \tau \mathbf{v_k} \mathbf{F} \frac{\partial f_0}{\partial E} = f_0 + e\tau \mathbf{v_k} \mathbf{E} \frac{\partial f_0}{\partial E}$$

$$\begin{aligned}\mathbf{J} &= -e \int \mathbf{v_k} dk_x dk_y dk_z \\ &= -e \int \mathbf{v_k} D(E) f(E) dE \\ &= -e \int \mathbf{v_k} D(E) \left[f_0 + e\tau \mathbf{v_k} \mathbf{E} \frac{\partial f_0}{\partial E}\right] dE \\ &= -e \int \mathbf{v_k} D(E) \left[e\tau \mathbf{v_k} \mathbf{E} \frac{\partial f_0}{\partial E}\right] dE\end{aligned}$$

$$J_x = -e^2 \int {v_x}^2 \tau(E) D(E) \frac{\partial f_0}{\partial E} dE \cdot E_x = -\frac{e^2}{k_B T} \int {v_x}^2 \tau(E) D(E) f_0 (1 - f_0) dE \cdot E_x$$

$$\frac{\partial f_0}{\partial E} = \frac{1}{k_B T} f_0 (1 - f_0)$$

Conductivity, relaxation time, mobility

$$\sigma_{xx} = -\frac{e^2}{k_B T}\int v_x{}^2 \tau(E) D(E) f_0(1-f_0)\,dE$$

$$= -\frac{2e^2}{3m_e^* k_B T}\int (E-E_0)\tau(E) D(E) f_0(1-f_0)\,dE$$

$$E - E_0 = \frac{1}{2}m_e^* \mathbf{v_k}{}^2 = \frac{3}{2}m_e^* \boldsymbol{v_x}{}^2$$

$$\sigma_{xx} = en\mu_{xx} = en\frac{e}{m_e^*}\langle\tau\rangle$$

$$n = \int D(E) f_0(E)\,dE$$

$$\langle\tau\rangle = -\frac{2e}{3}\int (E-E_0)\tau(E) D(E)\frac{\partial f_0}{\partial E}\,dE \Big/ \int D(E) f_0(E)\,dE$$

$$\mu_{xx} = \frac{e}{m_e^*}\langle\tau\rangle$$

Relaxation time approx.

Carrier density

$$n_e = \int_{E_C}^{\infty} D_C(E) f_e(E) dE$$

Conductivity and Mobility

$$\sigma_x = e n_e \boxed{\frac{e}{m_e^*}\left\langle \tau^1 \right\rangle} \rightarrow \mu_{drift}$$

$$\left\langle \tau^k \right\rangle = -\frac{2}{3}\int_{E_C}^{\infty} (E - E_m)\tau(E)^k D_C(E) \frac{\partial f_e(E)}{\partial E} dE \Big/ n_e$$

$$\tau(E,T) = \tau_0 T^p (E - E_m)^{r-1/2}$$

ex. $p = 0$, $r = 1/2$ for alloy scatt.)

Hall effect: Boltzmann equation

太田英二、坂田亮著、半導体の電子物性光学、培風館 (2005)

$$\boldsymbol{J} = \frac{e^2 n}{m_e^*}\left[\langle\frac{\tau}{1+(\omega_c\tau)^2}\rangle \boldsymbol{E} + \left(\frac{e}{m_e^*}\right)^2 \langle\frac{\tau^2}{1+(\omega_c\tau)^2}\rangle \boldsymbol{B}(\boldsymbol{B}\cdot\boldsymbol{E}) + \frac{e}{m_e^*}\langle\frac{\tau^2}{1+(\omega_c\tau)^2}\rangle \boldsymbol{E}\times\boldsymbol{B}\right]$$

When $B \cdot E = 0,\ \omega_c\tau \ll 1$

$$\boldsymbol{J} = en\mu\left[\langle\tau\rangle\boldsymbol{E} + \frac{e}{m_e^*}\langle\tau^2\rangle\boldsymbol{E}\times\boldsymbol{B}\right] = \sigma\left[\boldsymbol{E} + \frac{e}{m_e^*}\frac{\langle\tau^2\rangle}{\langle\tau\rangle}\boldsymbol{E}\times\boldsymbol{B}\right]$$

$$J_x = \sigma E_x + \sigma\mu\frac{\langle\tau^2\rangle}{\langle\tau\rangle^2}E_y B_z$$

$$J_y = \sigma E_y - \sigma\mu\frac{\langle\tau^2\rangle}{\langle\tau\rangle^2}E_x B_z = 0 \Rightarrow E_y = \frac{e}{m_e^*}\frac{\langle\tau^2\rangle}{\langle\tau\rangle}E_x B_z$$

$$J_z = \sigma E_z$$

$$E_y = -\frac{\frac{F_H\mu}{\sigma}B_z J_x}{1+(F_H\mu)^2 {B_z}^2} = -\frac{1}{en}B_z J_x$$

$$\boldsymbol{R_H = -\frac{V_H}{I_x}\frac{d}{B_z}}$$ **(for electron)**

$\boldsymbol{F_H = \frac{\langle\tau^2\rangle}{\langle\tau\rangle^2}}$**: Hall factor** $\boldsymbol{\mu_H = F_H\mu}$**: Hall mobility**

Hall effect

$R_H = F_{\text{Hall}} / qn$ $\quad$ $\boldsymbol{n_{Hall} = n_e / F_{Hall}}$

$\boldsymbol{\mu_{Hall} = \mu_{drift} F_{Hall}}$

Hall factor $\boldsymbol{F_{Hall} = \langle \tau^2 \rangle / \langle \tau^1 \rangle^2}$ $: 0.9 \sim 2$

$$\langle \tau^k \rangle = -\frac{2}{3} \int_{E_C}^{\infty} (E - E_m) \tau^k(E) D_C(E) \frac{\partial f_e(E)}{\partial E} dE / n_e$$

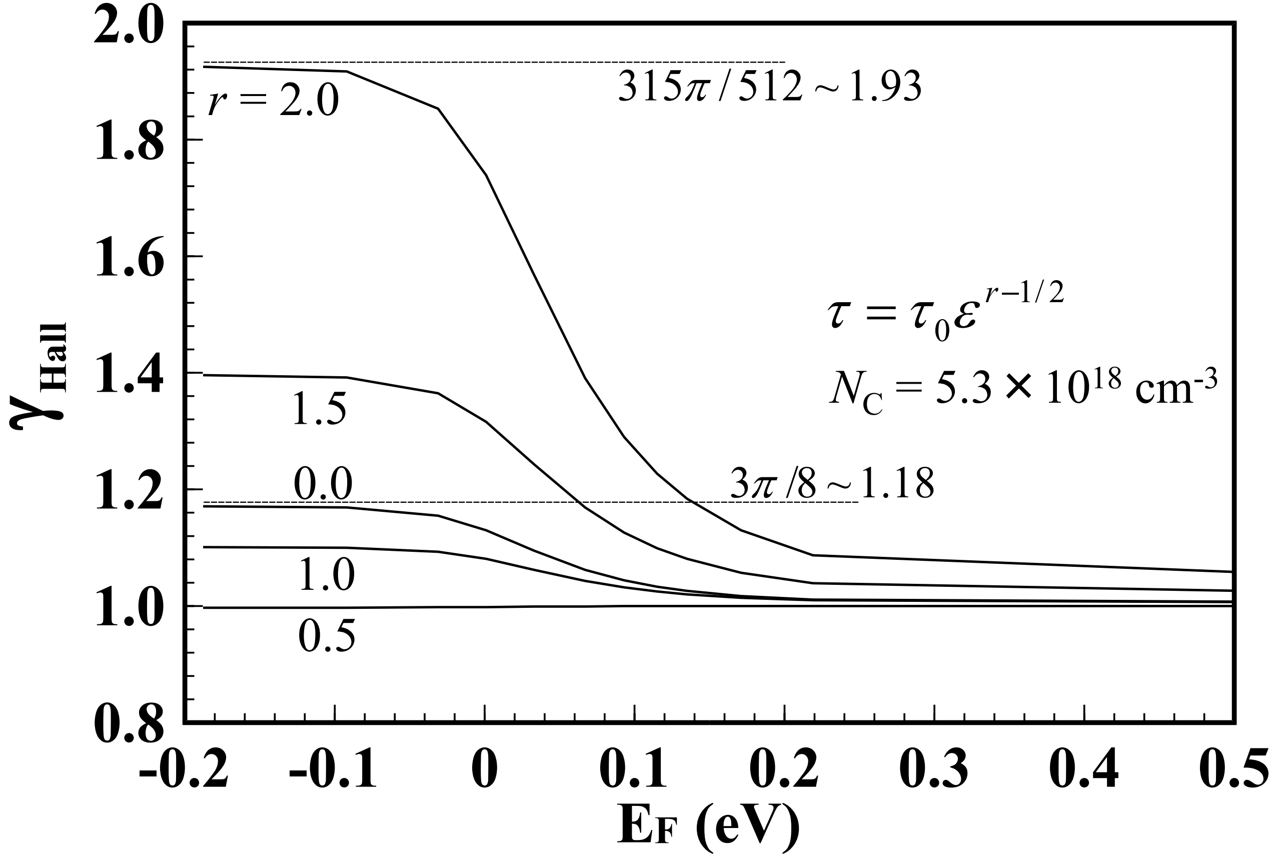
Energy-dependent relaxation time

=> Causes difference btw drift mobility and Hall mobility

Hall factor F_{Hall}

$R_H = F_{\text{Hall}} / qn$

F_{Hall}: determined by scattering mechanism



Different mobilities

- Drift mobility (definition)

  $\mu_d = E / v_{drift}$

  measured by time-of-flight methods

  Very thick film required

- Conductivity mobility

  $\mu_c = \sigma / (en)$: How to determine n?

- Hall mobility

  $V_H = R_H I_x B_Z / d$, $R_H = \gamma / en_{Hall}$

  $\mu_{Hall} = \sigma / (en_{Hall}) = \gamma\mu_d$

  ($\gamma = 1 - 2$: Hall factor, or scattering factor)

  DC mobility including grain boundary effects

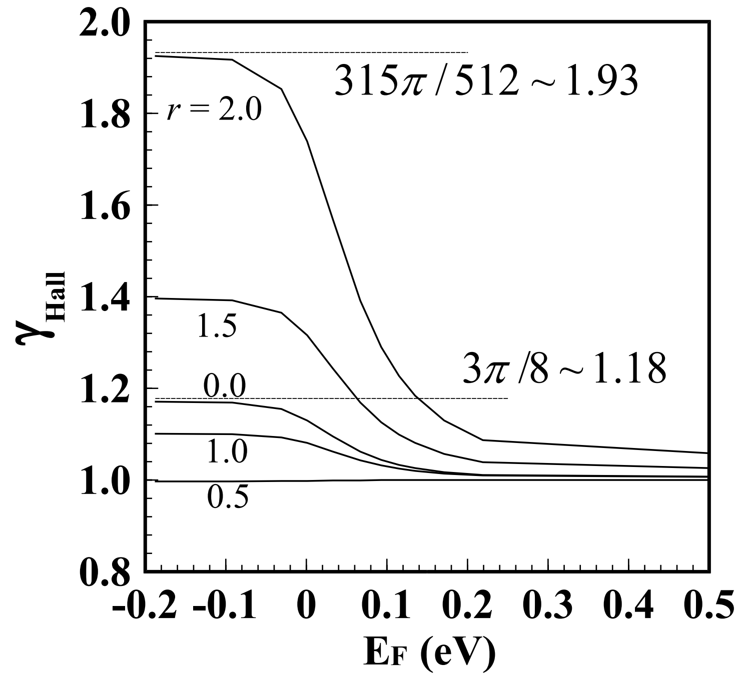
- Optical mobility

  From free carrier absorption

  High-doping required, Local mobility

- Field-effect mobility

  Largely depends on quality of TFT / FET



Known from effective mass (free e^- approx.)

Mobility, conductivity $\mu = \frac{e\tau}{m_e^*}$ $\sigma = eN_{free}\mu$

Density of state function M_C is the degeneracy of LUMO

$$N(E) = M_C \frac{\sqrt{2}}{\pi^2} \frac{\sqrt{E - E_C}}{\hbar^3} m_{de}^{3/2}$$

Burstein-Moss shift
(E_F of degenerated semiconductor) $\Delta E_g^{BM} = \frac{h^2}{m_{de}} \left(\frac{3N_e}{16\sqrt{2}\pi} \right)^{2/3}$

Effective density of state N_C, N_V

for isotropic CBM/VBM that does not have extra degeneracy other than spin, density-of-states effective mass m_{de} is equal to carrier effective mass m_e^*.

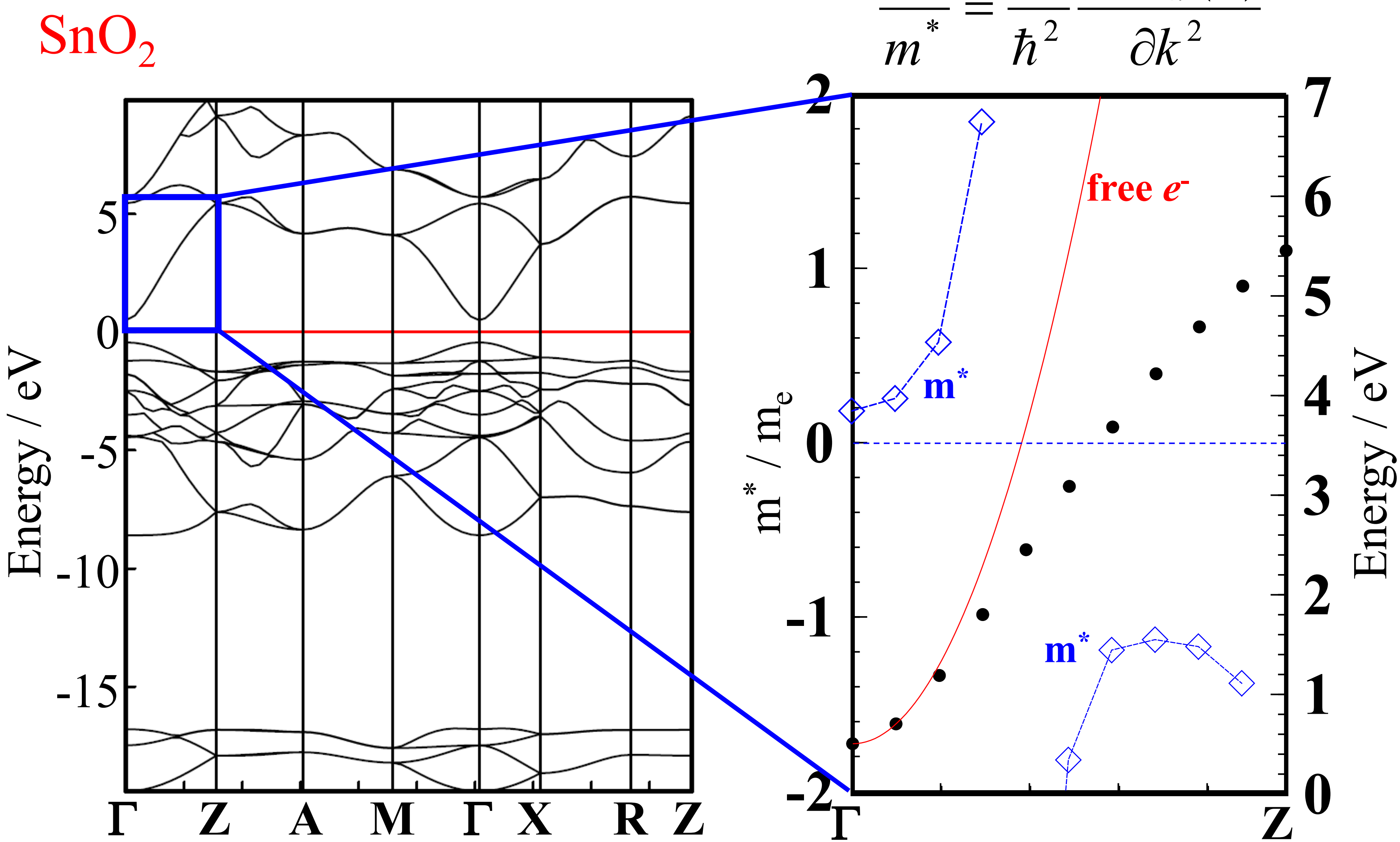
$$N_C = 2\left(\frac{2\pi m_{de} k_B T}{h^2} \right)^{3/2} M_C$$

Thermal velocity $\frac{1}{2} m_e^* v_{th}^2 = \frac{3}{2} k_B T$ $v_{th} = \sqrt{3k_B T / m_e^*}$

Fermi velocity $\frac{1}{2} m_e^* v_F^2 = E_F - E_C$ $v_F = \sqrt{2(E_F - E_C)/ m_e^*}$

Effect on m_e^*: Band effective mass

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 E_n(\mathbf{k})}{\partial k^2}$$



Effect on m_e^*: Electron-lattice interaction

Electrons interact with host ions => Larger effective mass

=> Polaron

Weak interaction, electrons are not localized: Large polaron

Strong interaction, electorns are localized in unit cell: Small polaron

Frölich polaron model

$$m^* = m_0^*(1 + \alpha/6 + \cdots)$$

$$\alpha = \frac{e^2}{8\pi\varepsilon_0\hbar^2}\sqrt{\frac{2m^*}{\hbar\omega}}\left(\frac{1}{\varepsilon_{r\infty}-\varepsilon_{rs}}\right)$$

0.068 for GaAs

3.8 for $SrTiO_3$

H. Frolich: Adv. Phys. 1954, 3, p. 325.

Termoelectrics

熱起電力

Thermoelectricity: Boltzmann equation

太田英二、坂田亮著、半導体の電子物性光学、培風館 (2005)

Boltzmann-Bloch equation

$$\frac{df(\boldsymbol{k})}{dt} = -\frac{\boldsymbol{F}}{\hbar}\frac{\partial f(\boldsymbol{k})}{\partial \boldsymbol{k}} - \boldsymbol{v}_{\boldsymbol{k}}\frac{\partial f(\boldsymbol{k})}{\partial \boldsymbol{r}} - \frac{f(\boldsymbol{k}) - f_0(\boldsymbol{k})}{\tau(\boldsymbol{k})}$$

$\boldsymbol{v}_{\boldsymbol{k}} = \frac{d\varepsilon(\boldsymbol{k})}{d\boldsymbol{k}}$: group velocity ⇔ $\boldsymbol{v}_{\boldsymbol{p}} = \frac{\varepsilon(\boldsymbol{k})}{\boldsymbol{k}}$: phase velocity

Steady-state $\frac{df(\boldsymbol{k})}{dt} = -\frac{\boldsymbol{F}}{\hbar}\cdot\frac{\partial f(\boldsymbol{k})}{\partial \boldsymbol{k}} - \boldsymbol{v}_{\boldsymbol{k}}\cdot\frac{\partial f(\boldsymbol{k})}{\partial \boldsymbol{r}} - \frac{f(\boldsymbol{k}) - f_0(\boldsymbol{k})}{\tau(\boldsymbol{k})} = 0$

Non-uniform T and chemical potential η: depend on position $\boldsymbol{r}$

$$f(\boldsymbol{k}) - f_0(\boldsymbol{k}) = -\tau(\boldsymbol{k})\left(\frac{\boldsymbol{F}}{\hbar}\cdot\frac{\partial f(\boldsymbol{k})}{\partial \boldsymbol{k}} + \boldsymbol{v}_{\boldsymbol{k}}\cdot\frac{\partial f(\boldsymbol{k})}{\partial \boldsymbol{r}}\right)$$

$$= -\tau(\boldsymbol{k})\left(e\boldsymbol{E}\cdot\frac{\partial\varepsilon(\boldsymbol{k})}{\partial \boldsymbol{k}}\frac{\partial f(\varepsilon)}{\partial\varepsilon} + \boldsymbol{v}_{\boldsymbol{k}}\cdot T\nabla\frac{\varepsilon-\eta}{T}\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right)$$

$$= -\tau(\boldsymbol{k})\frac{\partial f(\varepsilon)}{\partial\varepsilon}\boldsymbol{v}_{\boldsymbol{k}}\cdot\left(e\boldsymbol{E} + T\nabla\frac{\varepsilon-\eta}{T}\right)$$

Thermoelectricity: Boltzmann equation

太田英二、坂田亮著、半導体の電子物性光学、培風館 (2005)

$$\boldsymbol{J} = en\frac{\int (\boldsymbol{v_k}\otimes\boldsymbol{v_k})\tau(\boldsymbol{k})\left(-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right)\left[e\boldsymbol{E}+T\nabla\frac{\varepsilon-\eta}{T}\right]d\boldsymbol{k}}{\int f_0(\boldsymbol{k})d\boldsymbol{k}}$$

$(\boldsymbol{v_k}\otimes\boldsymbol{v_k}) = (v_{k,i}v_{k,j})$: Direct product of vectors

$$\nabla\frac{\varepsilon-\eta}{T} = -\frac{\varepsilon-\eta}{T}\nabla T - \nabla\eta$$

Chemical potential η is a function of carrier density $n(r)$

$$\boldsymbol{J} = \sigma\cdot\boldsymbol{E} + en\frac{\langle\tau\rangle}{m_e^*}\left[\frac{1}{T}\left(\frac{\langle\tau\varepsilon\rangle}{\langle\tau\rangle} - \eta + T\frac{\partial\eta}{\partial T}\right)\nabla T + \frac{\partial\eta}{\partial n}\nabla \mathrm{n}\right]$$

$$= \sigma\cdot\boldsymbol{E} + \sigma\left[S\nabla T + \frac{1}{e}\frac{\partial\eta}{\partial n}\nabla \mathrm{n}\right]$$

$$\boldsymbol{S} = \frac{\mathbf{1}}{\boldsymbol{eT}}\left[\left(\frac{\langle\boldsymbol{\tau\varepsilon}\rangle}{\langle\boldsymbol{\tau}\rangle} - \boldsymbol{\eta} + \boldsymbol{T}\frac{\boldsymbol{\partial\eta}}{\boldsymbol{\partial n}}\right)\right]$$

Seebeck coefficient

$$\boldsymbol{S = \frac{1}{eT}\left[\left(\frac{\langle\tau\varepsilon\rangle}{\langle\tau\rangle} - \eta + T\frac{\partial\eta}{\partial n}\right)\right]}$$

$$S = -\frac{k}{e}\frac{\int \left(-\frac{\partial f}{\partial E}\right)D(E)v^2\tau\left[\frac{E-E_F}{kT}\right]dE}{\int \left(-\frac{\partial f}{\partial E}\right)D(E)v^2\tau dE} + \frac{1}{e}\frac{\partial E_F}{\partial T}$$ Seebeck coefficient

$$\tau = (m_e^*/2)^{1/2} l_0(T) E^{r-1/2}$$

Degenerated semi.: Free-electron like, single band, $\tau=\tau_0+((E-E_F)/E_F)\,\tau_1$

$$S \sim -\frac{k}{e}\frac{\pi^2}{3}\left(\frac{3}{2}+\frac{\tau_1}{\tau_0}\right)\frac{kT}{E_F}$$

Non-degenerated band:

$$S \sim -\frac{k}{e}\left(\frac{E_C - E_F}{kT} + r + 2\right) = -\frac{k}{e}\left(\ln\frac{N_C}{N_e} + r + 2\right)$$ Electrons

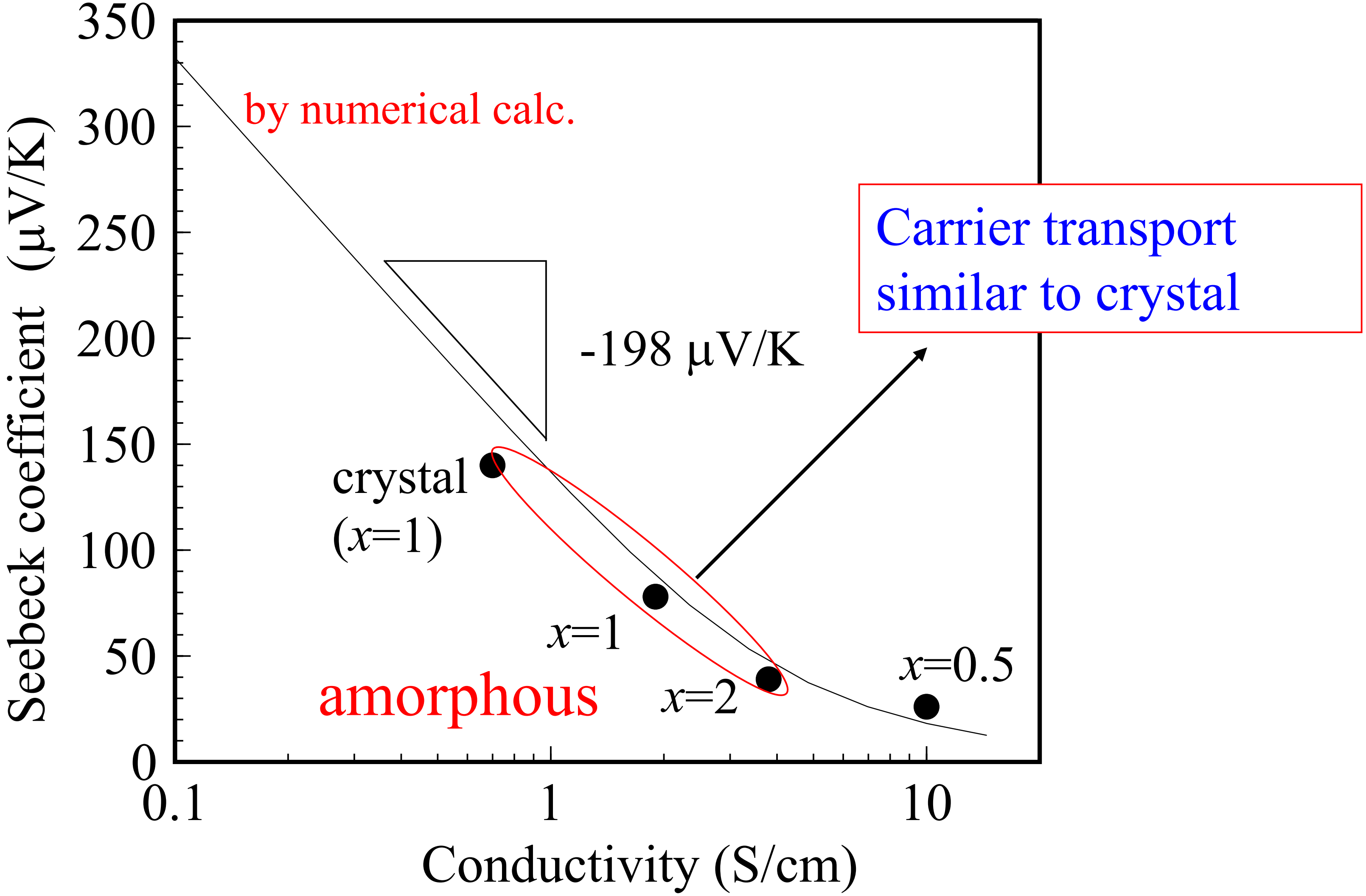
$$S \sim +\frac{k}{e}\left(\frac{E_F - E_V}{kT} + r + 2\right) = +\frac{k}{e}\left(\ln\frac{N_V}{N_h} + r + 2\right)$$ Holes

Hopping conduction (small polaron): Entropy S

$$S = \frac{k}{e}\ln\left(\frac{n}{N-n}\right)$$

Jonker plot: ex. For p-type xZnO·Rh_2O_3

$n = \sigma / \mu / e$ ⇨ $S = -\frac{k}{e}(\log\sigma - \log\mu_h + A)$ $\frac{k}{e} = 198\mu V/K$



G.H. Jonker, Philips Res. Repts 23 (1968) 131; Kamiya et al., Adv. Funct. Mater. 15, 968 (2004)

Mott formula

$c(E) = e^2 N(E) D(E)$: Energy-dependent conductivity

$N(E)$: Density of states

$D(E)$: Electron diffusion constant

$= \mu kT/e$: Einstein's relation

Boltzmann equation

$$\sigma_{xx} = -e^2 \int v_x{}^2 \tau(E) N(E) \frac{\partial f_0}{\partial E} dE$$

$$= \int c(E) \left[-\frac{\partial f(E)}{\partial E} \right] dE$$

$$\sigma S = -\frac{k}{e} \int \frac{E-\mu}{kT} c(E) \left[-\frac{\partial f(E)}{\partial E} \right] dE$$

Seebeck sign anomary for localized e^-

VRH conduction of localized e^-

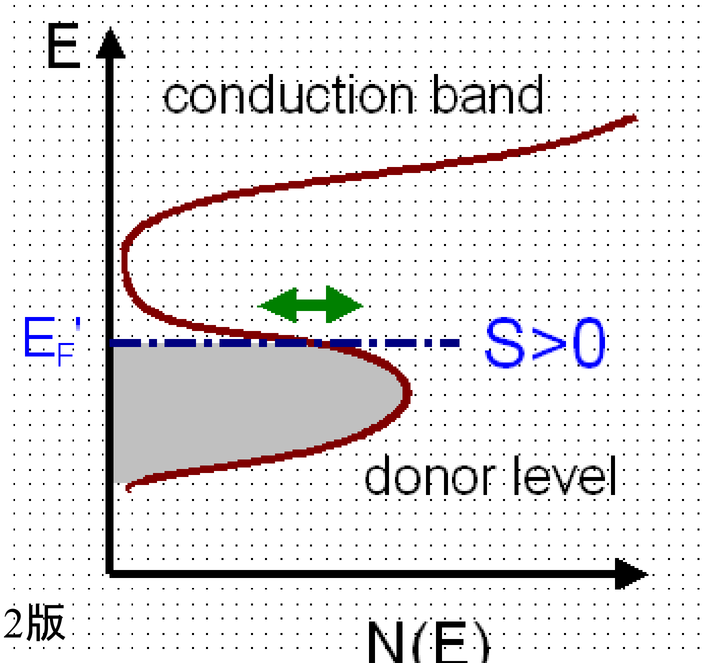
Mott's formula: $S = \frac{\pi^2}{3}\frac{k_B{}^2 T}{e}\left(\frac{d\ln\sigma(E)}{dE}\right)_{E=E_F}$

$\sigma(E) = e^2 D(E) D_{diff}$ D_{diff}: Electron diffusion constant

$$S = \frac{1}{2}\frac{k_B}{e}\frac{W^2}{k_B T}\left(\frac{d\ln D(E)}{dE}\right)_{E=E_F} = \frac{1}{2}\frac{k_B{}^2}{e}(T_0 T)^{1/2}\left(\frac{d\ln N(E)}{dE}\right)_{E=E_F}$$

$$W = k_B\left(T_0 T^3\right)^{1/4}$$

Suppose equal to hopping activation energy



I.P. Zvyagin, Phys. Stat. Sol. B58 (1973) 443
V.V. Kosarev, Sov. Phys. – Semicond. 8 (1975) 897
H. Overhof, Pys. Stat. Sol. B67 (1975) 709
P. Butcher, in Proc. 6th ICALS (1976) p.89
「非晶質材料の電気伝導」、ネビルモット著、現代工学社、2003年第2版

Measurement of electrical conductivity and mobilities

電気伝導度･移動度の測定

Measurement of electrical conductivity

$V = RI$

R [Ω]: resistance

$I = GV$

G [S/cm]: conductance

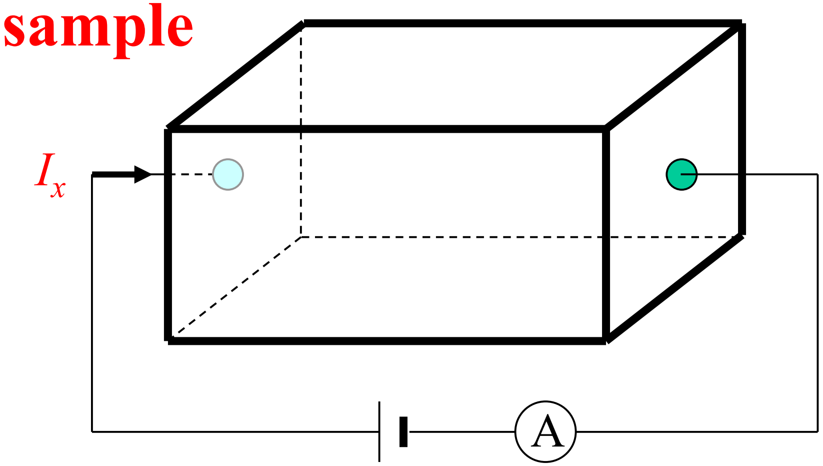
$E = \rho J$

ρ [Ωcm]: resistance

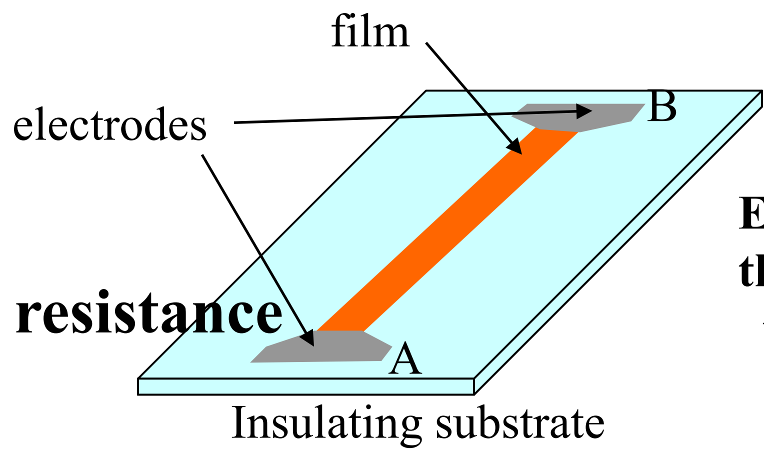
$J = \sigma E$

σ: conductivity

Bulk sample



Film sample



Electrode W, L
thickness t
t << W, L

$\rho = R\frac{S}{d}$

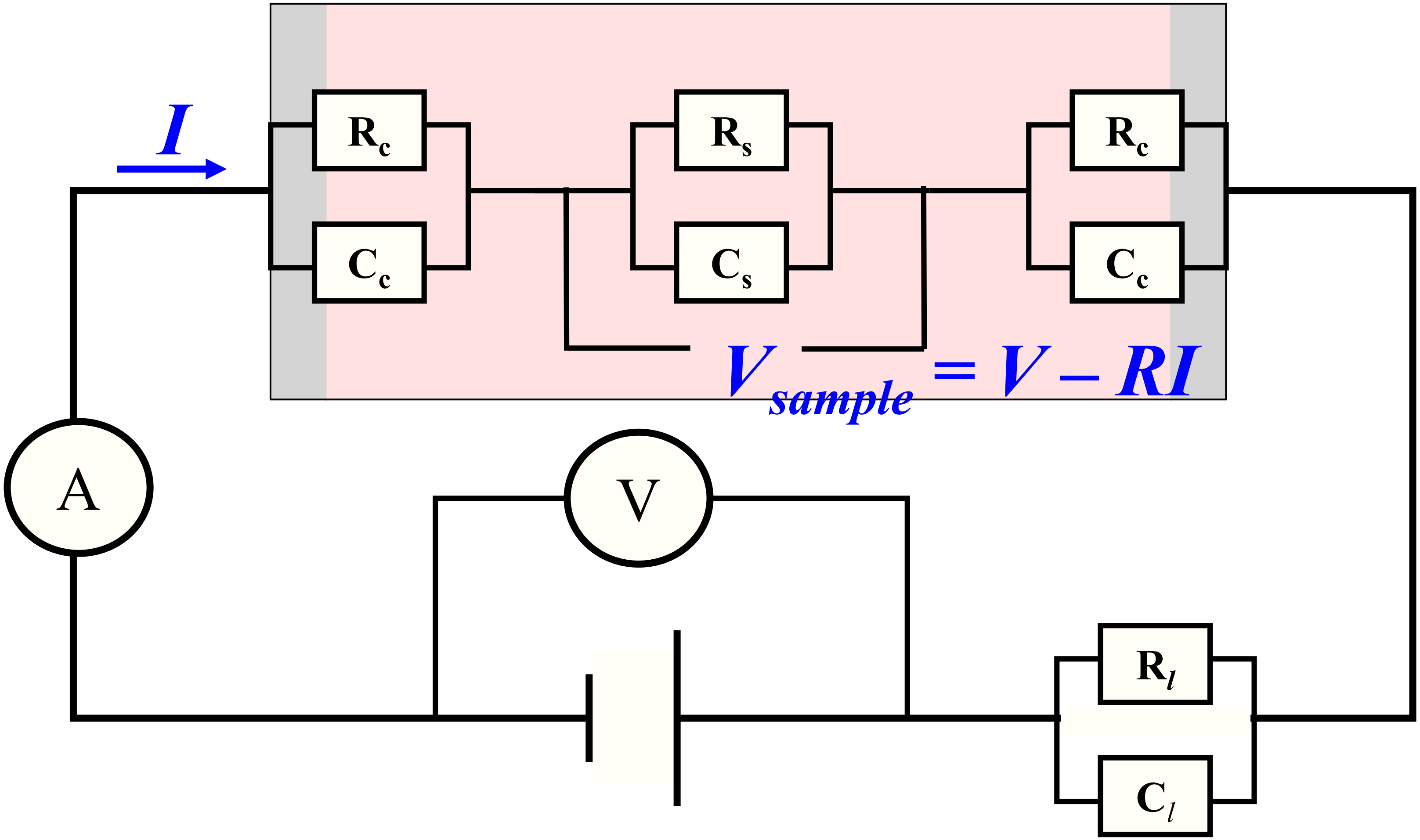
$R_s = \rho/t$ [Ω/□, Ω□]: sheet resistance

$\sigma = G\frac{d}{S}$

$\sigma_s = \sigma t$ [S/□, S□]: sheet conductance

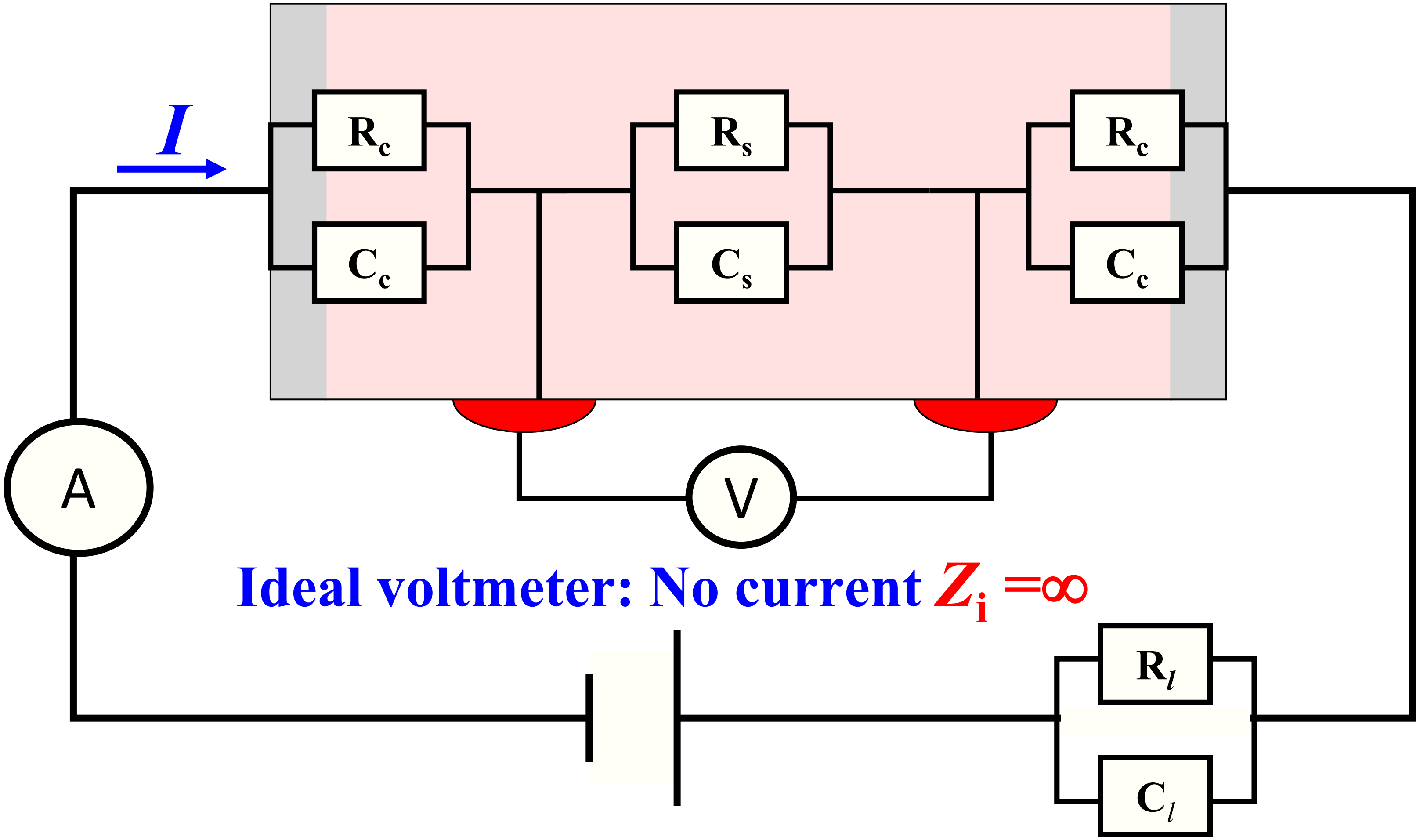
Two-terminal method may take extra resistances from electrodes and interfaces

May over estimate resistivity for low-R samples



Extra resistance effects are reduced for four-terminal method

Input impedance of voltmeter Z_i >> Sample impedance Z_s

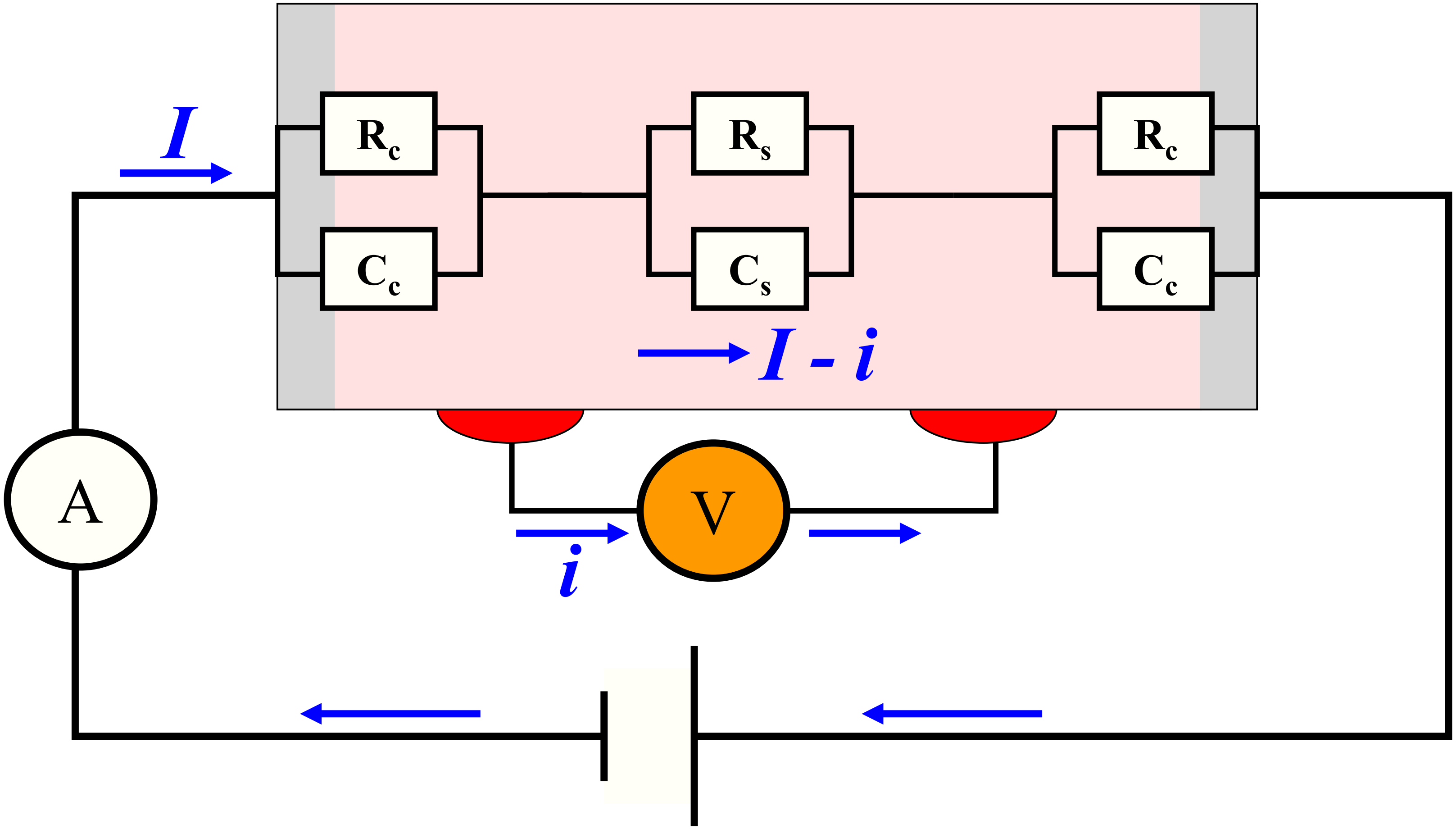


Ideal voltmeter: No current $Z_i = \infty$

Very high resistance sample

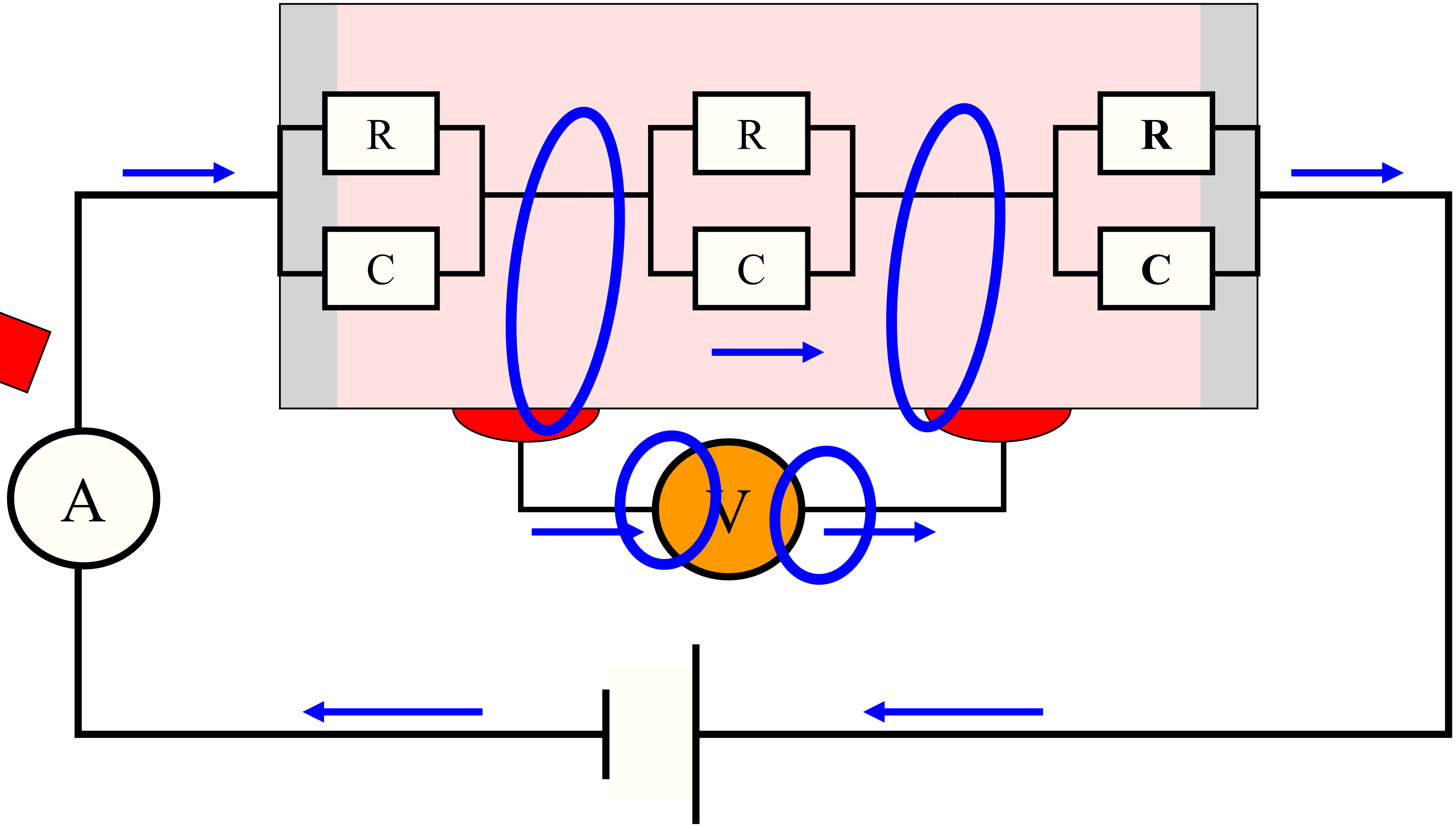
$Z_i >> Z_s$

- Usual voltmeter like DMM (e.g.,Keithley 2001, $Z_i \sim 100M\Omega$):
  Current loss through V-meter
- Very high Z_i V-meters: Electrometer, picoammeter (e.g., Keithley 6517)



Extremely high resistance sample

- Current loss even through electrometer
- If electric capacitances are formed at the V-meter – sample interface, it causes voltae drop



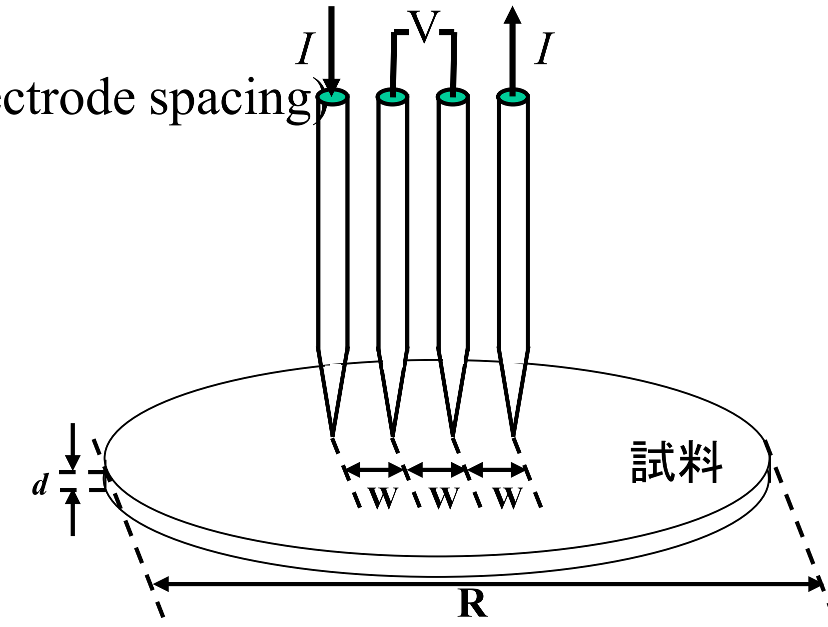
Four-probe method

Easy, convenient, non-destructive, no electrode
Sample size *R* and thickness *t* should be >> *W* (electrode spacing)
For bulk sample,

$$\rho = 2\pi W\ (V/I)$$

If *d* is small enough compared to *W*

$$\rho = Cd(V/I)$$



Shape factor *C*

R/W	*C*	R/W	*C*
3.0	2.2662	20.0	4.4364
4.0	2.9289	40.0	4.5076
5.0	3.3625	∞	$\pi / \ln 2 = 4.5324$
10.0	4.1716		

I.B. Valdes, Proc. IRE **42**, 420 (1954)
F.M. Smits, The Bell System Technical Journal **37**, 711 (1958)
S. Murashima, F. Ishibashi, Jpn. J. Appl. Phys. **9**, 1340 (1970)]

Van der Pauw method

L.J. van der Pauw, Philips. Res. Rep. **13** (1958) 1.

Apply current I_{AB}, measure V_{CD}

$$R_{AB,CD} = V_{CD} / I_{AB}$$

Apply current I_{BC}, measure V_{DA}

$$R_{BC,DA} = V_{DA} / I_{BC}$$

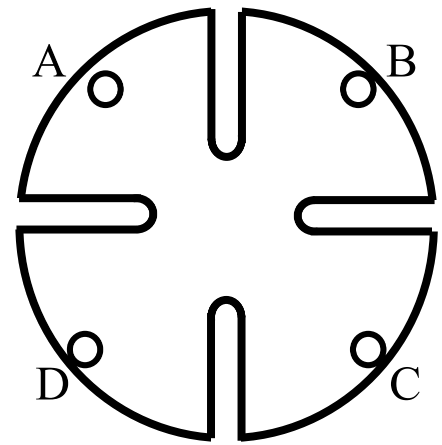
Apply B_z and I_{BC}, measure V_{BD}

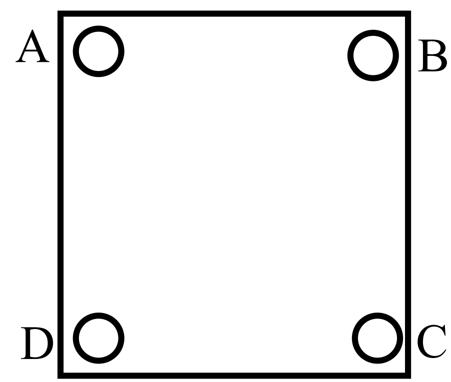
$$\triangle R_{AC,BD} = V_{BD} / I_{AC}$$

$$\rho = \frac{\pi d}{\ln 2} \cdot \frac{(R_{AB,CD} + R_{BC,DA})}{2} \cdot f(R)$$

$$n = \frac{B}{q \cdot d \cdot \triangle R_{AC,BD}} \qquad \mu_{\mathrm{Hall}} = \frac{d}{B_z} \cdot \frac{\triangle R_{AC,BD}}{\rho}$$

***f*(*R*): Shape factor** $\frac{\exp(\ln 2 / f)}{2} = \cosh\left\{\frac{\ln 2}{f}\frac{R-1}{R+1}\right\}$





Shape factor of van der Pauw method *f*

$R_{AB,CD} / R_{BC,DA}$	f	$R_{AB,CD} / R_{BC,DA}$	f
1.0	1.0	1.4	0.9903
1.1	0.9992	1.5	0.9860
1.2	0.9971	2.0	0.9603
1.3	0.9941	3.0	0.9067

van der Pauw method

L.J. van der Pauw, A method of measureing specific resistivity and Hall effect of discs of arbitrary shape, Phil. Res. Repts., **13**, 1 (1958)

It will be shown that the specific resistivity and the Hall effect of a flat sample of arbitrary shape can be measured without knowing the current pattern if the following conditions are fulfilled:

(a) The contacts are at the circumference of the sample.

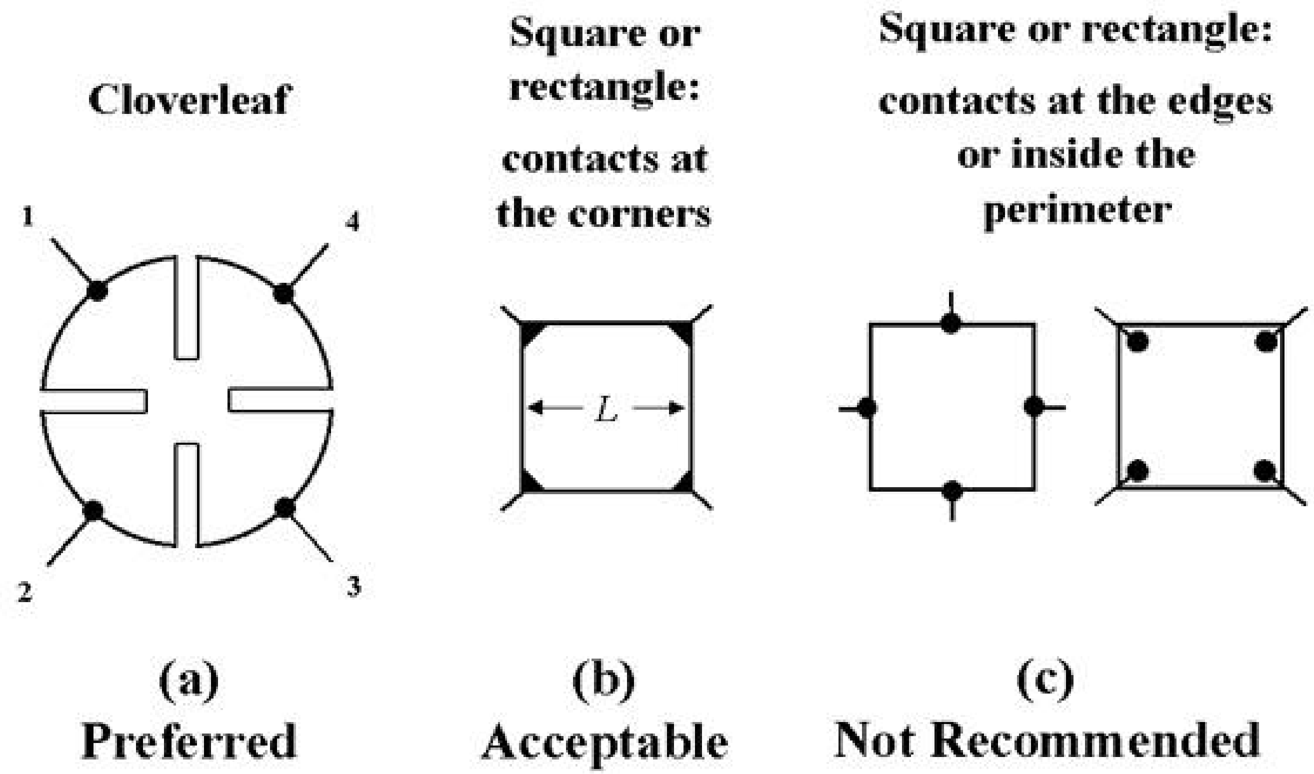
(b) The contacts are sufficiently small.

(c) The sample is homogeneous in thickness.

(d) The surface of the sample is singly connected, i.e., the sample does not have isolated holes.

Van der Pauw method

Geometry of electrodes

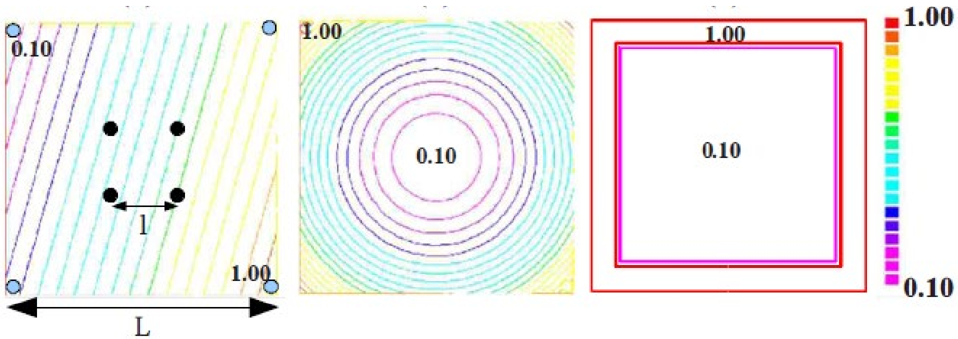


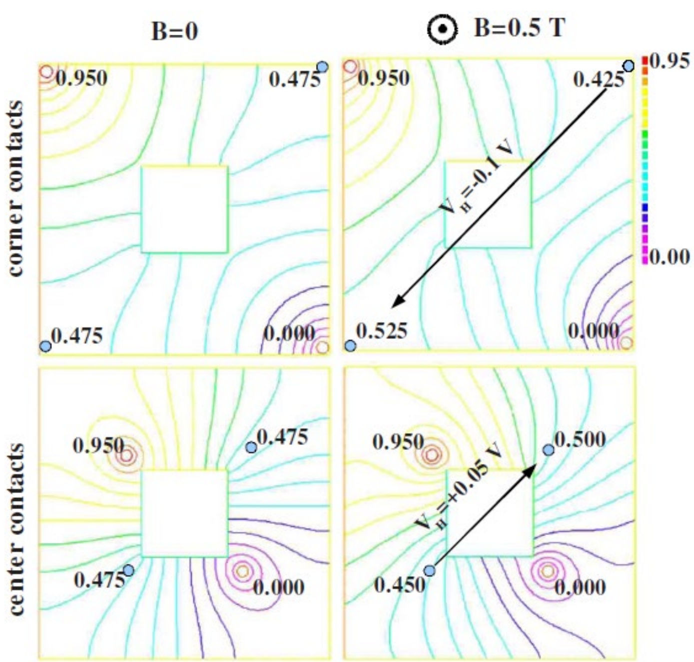
Apparent V_H anomaly in van der Pauw method

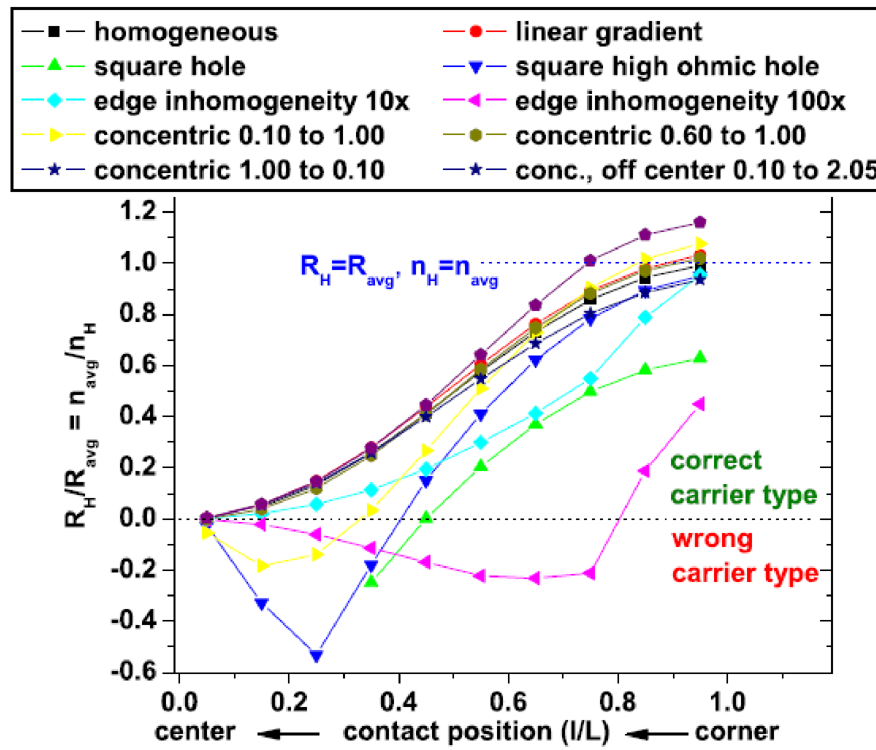
Causes of incorrect carrier-type identification in van der Pauw–Hall measurements

Oliver Bierwagen,[a] Tommy Ive, Chris G. Van de Walle, and James S. Speck

APPLIED PHYSICS LETTERS **93**, 242108 (2008)







Positive Hall coefficients obtained from contact misplacement on evident *n*-type ZnO films and crystals

Takeshi Ohgaki,[a] Naoki Ohashi, Shigeaki Sugimura,[b] Haruki Ryoken, Isao Sakaguchi, Yutaka Adachi, and Hajime Haneda

J. Mater. Res., 23 (2008) 2293

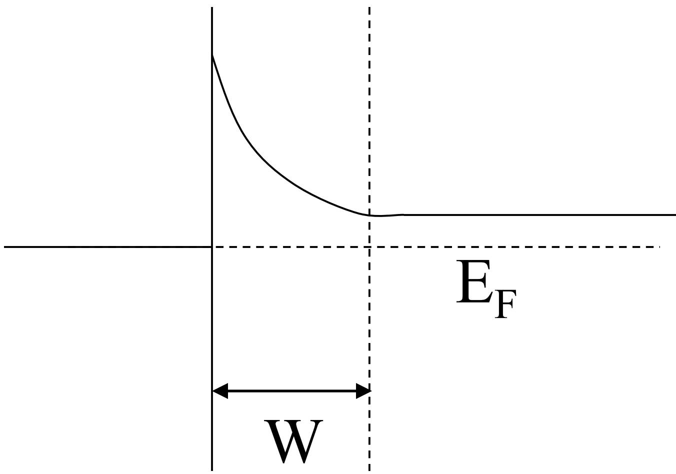
Impedance methods

インピーダンス測定

C-V method: Potential distribution in Schottky junction

Poisson equation $\frac{d^2V}{dx^2} = e\frac{N_D}{\varepsilon_s}$

$$V = ax^2 + bx + c \qquad \left.\frac{dV}{dx}\right|_{x=W} = 0$$



$$V(0 \le x \le W) = \frac{eN_D(x-W)^2}{2\varepsilon_s}$$

$$V_{bi} = V(0) - V(W) = \frac{eN_D W^2}{2\varepsilon_s}$$

Width of depletion layer $W = \left(\frac{2\varepsilon_s}{eN_D}(V_{bi} - V)\right)^{1/2}$

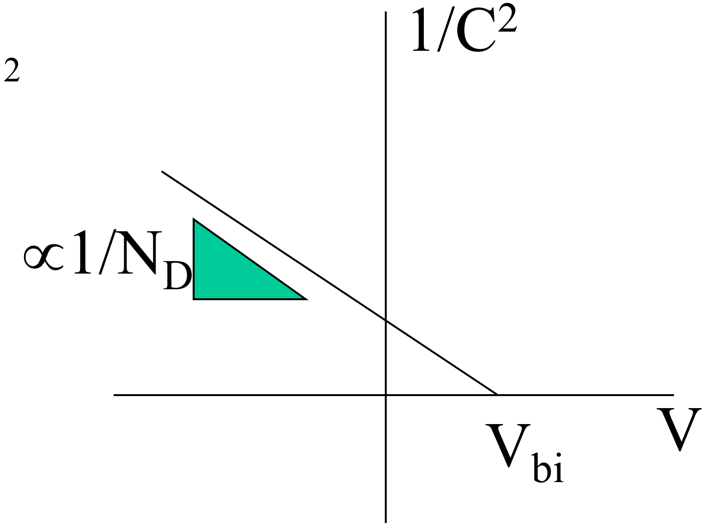
$$V_{bi} = \frac{\phi_m - \phi_s}{e}$$

ϕ_m, ϕ_s are work functions of the metal and the semiconductor

C-V method: Carrier polarity, N_D,V_{bi}

Charge in the depletion layer

$$Q_{sc} = eN_D W = eN_D \left(\frac{2\varepsilon_s}{eN_D} (V_{bi} - V) \right)^{1/2}$$



Junction capacitance = depletion layer cap.

$$C = \frac{dQ_{sc}}{dV} = \left(\frac{e\varepsilon_s N_D}{2(V_{bi} - V)} \right)^{1/2} = \frac{\varepsilon_s}{W}$$

$$\frac{1}{C^2} = \frac{2}{e\varepsilon_s N_D} (V_{bi} - V)$$

Carrier polarity: the sign of slope

V_{bi}: V-axis crosssection

N_D: Slope

For distributed $N_D(x)$

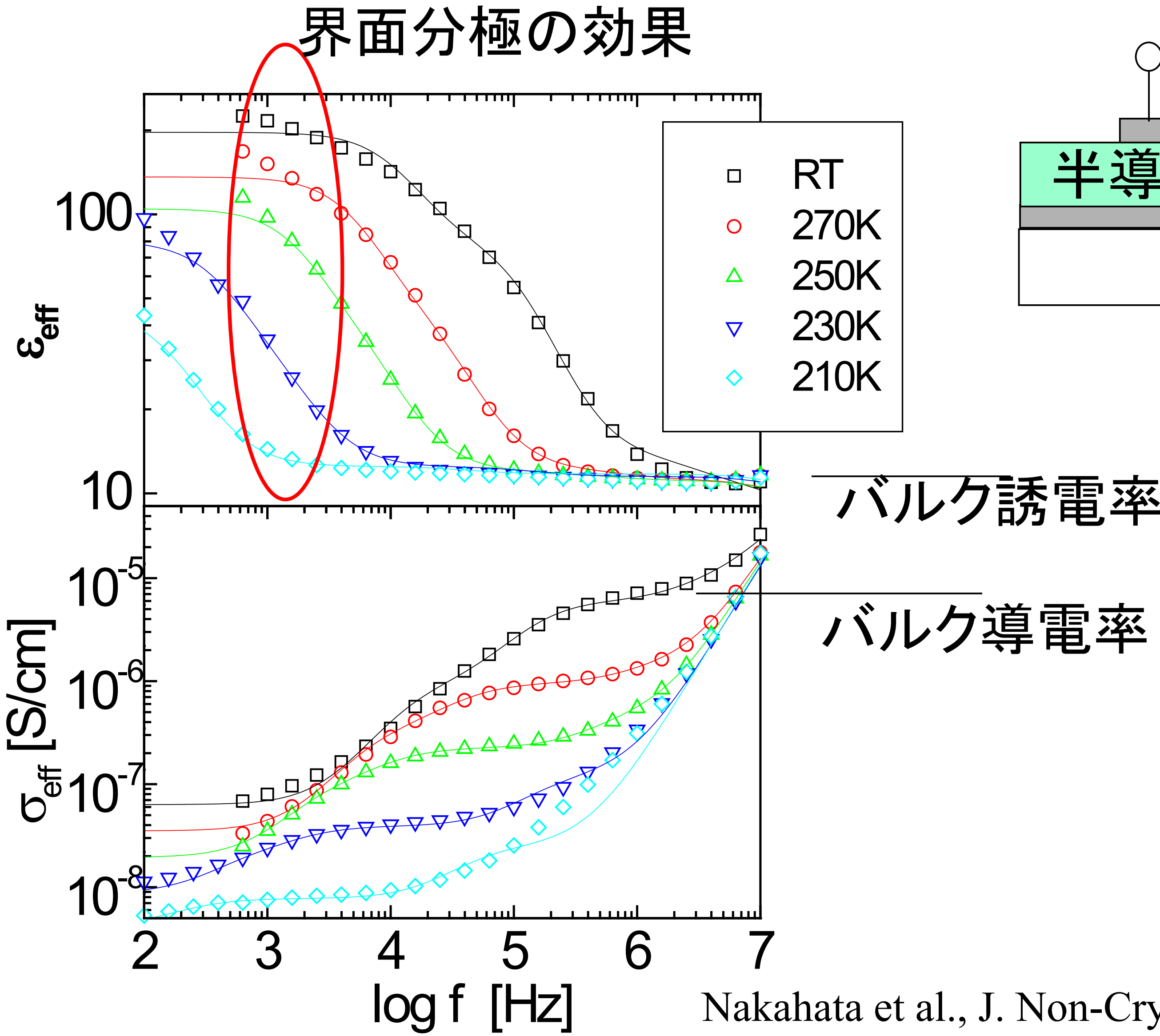
$$N_D(W) = \frac{2}{e\varepsilon_s} \left(\frac{dC^{-2}}{dV} \right)^{-1} = \frac{2C^3}{e\varepsilon_s} \left(\frac{dC}{dV} \right)^{-1}$$

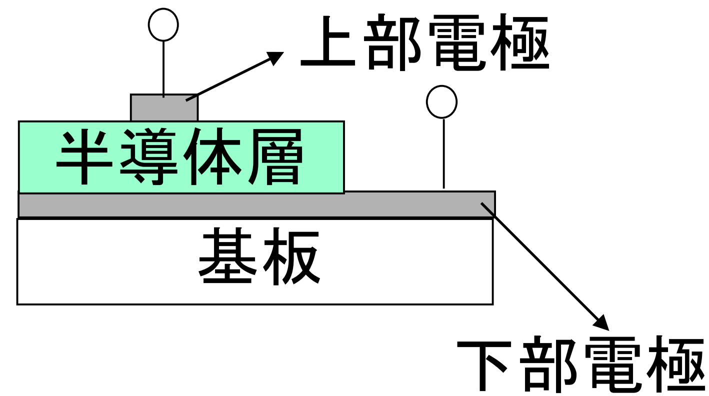
$$W = \varepsilon_s / C$$

半導体評価技術

河東田 隆 編著

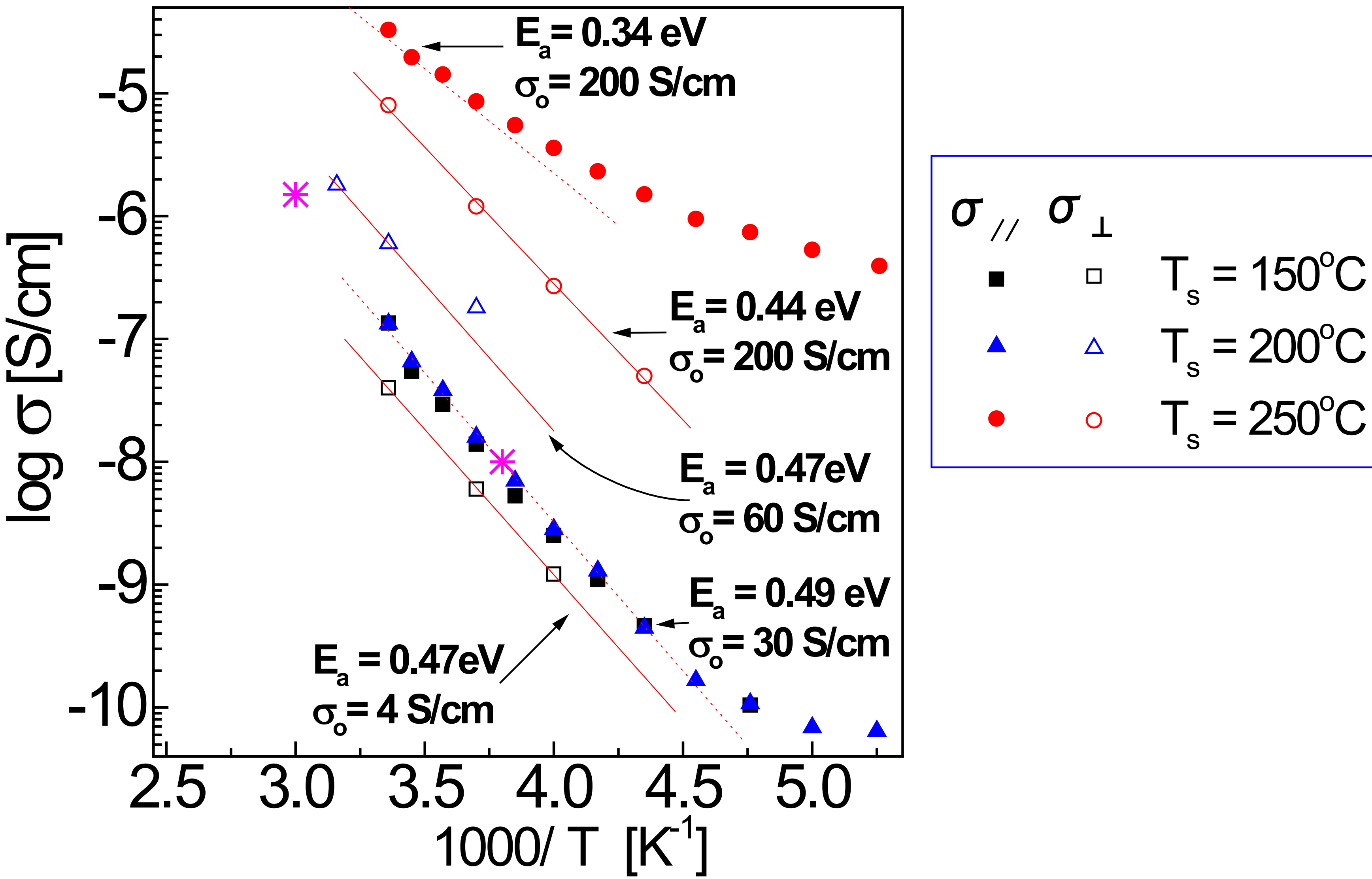
交流インピーダンス法による
縦方向薄膜伝導度測定





Nakahata et al., J. Non-Cryst. Sol. **266-269**, 120 (2000)

Arrhenius plot of conductivities perpendicular and parallel to film surface as a function of Ts

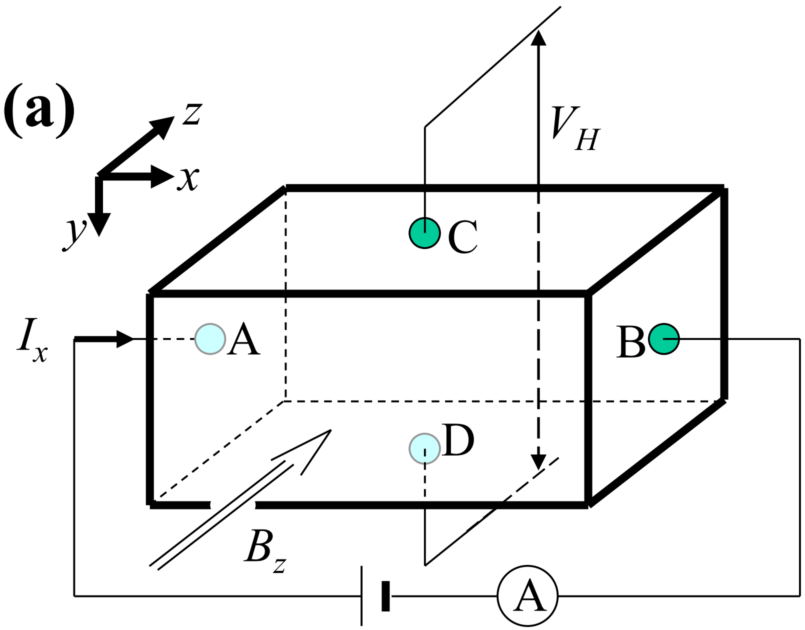


Hall effect

Hall効果

Six-terminal Hall bar

(a)



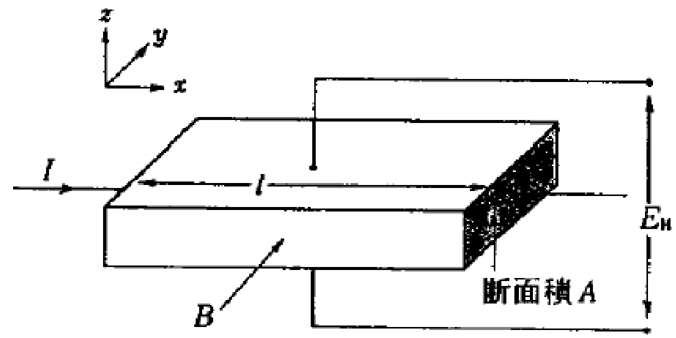
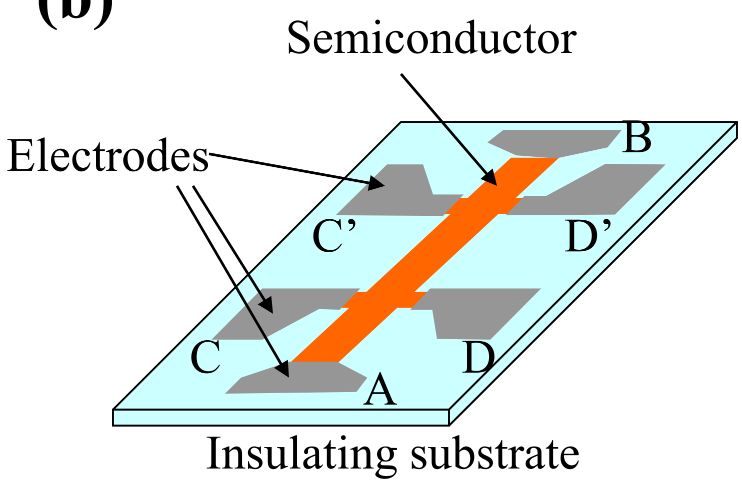


図 3·24 Hall 効果の実験

Measure resistivity by two-terminal method

(b)



- **Require pattering**
- **Can specify the transport path and direction**
- **Resistivity measured by four-terminal method**
- **Better accuracy by different electrode combinations**

Compensation of geometrical error by flipping *B* and *I*

If Hall voltage electrodes are mis-aligned:

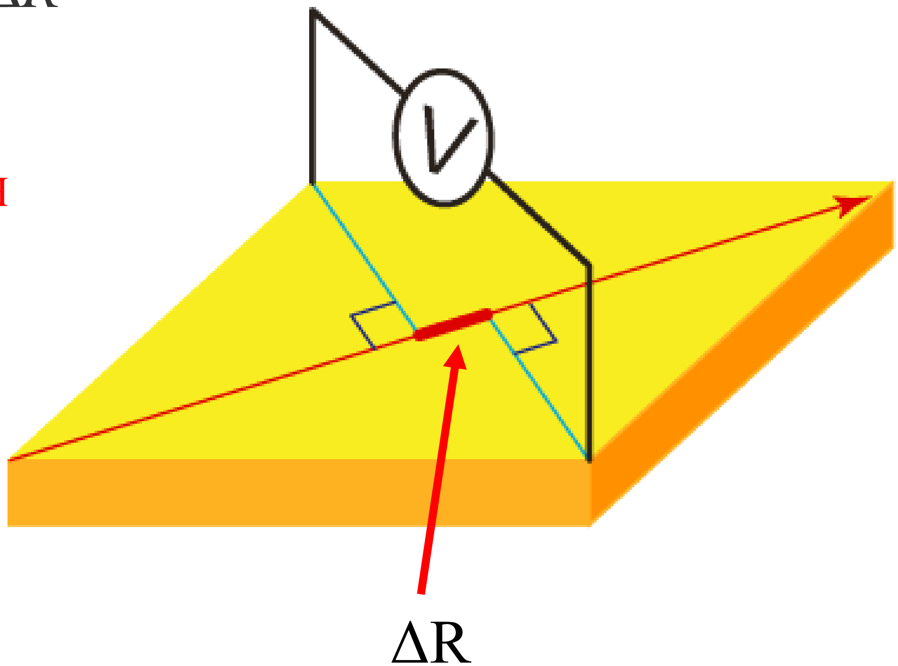
Hall voltage overestimate by the sample ΔRI

$$V_{obs}^{+} = BIR_{Hall}/t + I\Delta R$$

Flip *B*

$$V_{obs}^{-} = -BIR_{Hall}/t + I\Delta R$$

=> $(V_{obs}^{+} - V_{obs}^{-})/2 = -BIR_H$

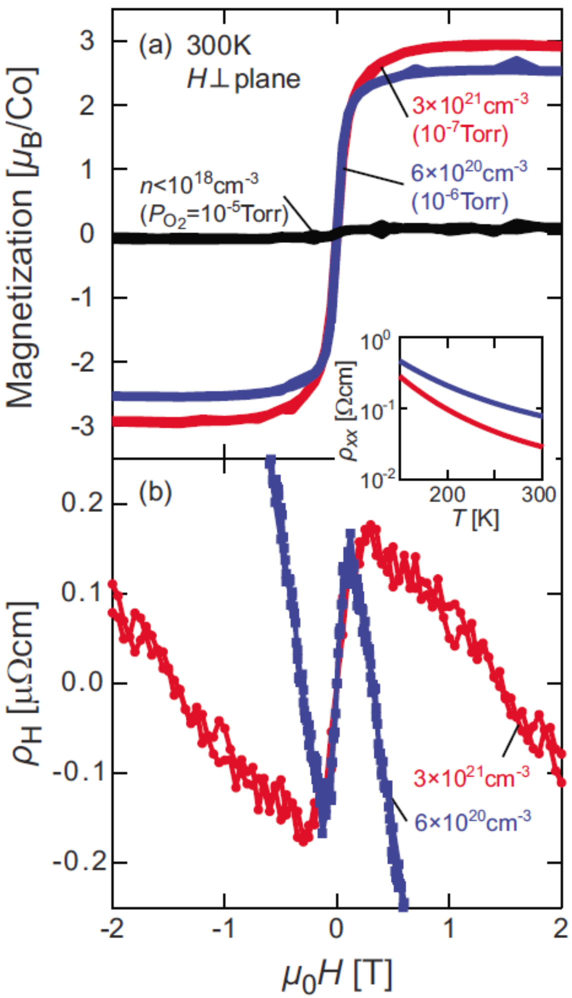


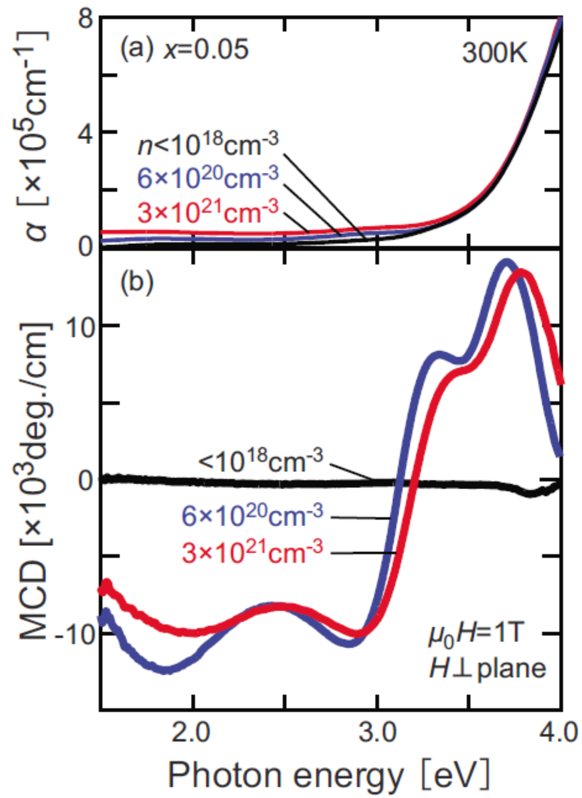
Anomalous Hall effect

Co-doped TiO_2 films grown on glass: Room-temperature ferromagnetism accompanied with anomalous Hall effect and magneto-optical effect

T. Yamasaki,[1] T. Fukumura,[1,2,a)] Y. Yamada,[1] M. Nakano,[1] K. Ueno,[3] T. Makino,[3] and M. Kawasaki[3,1,4]

APPLIED PHYSICS LETTERS **94**, 102515 (2009)





Optical mobility

光学移動度

Free carrier absorption and optical conductivity

Optical absorption by free carriers with the density *n*

$$m^* \frac{d^2x}{dt^2} + \frac{m^*}{\tau}\frac{dx}{dt} = qE$$

$$D = \varepsilon_0 E + P = \varepsilon_0 E + qNx = \varepsilon E$$

$$E = E_0 \exp(i\omega t)$$

$$\mu = \frac{m^* q}{\tau}$$

$$\begin{cases} \varepsilon_1 = n_f^{\,2} - k_f^{\,2} = \varepsilon\left(1 - \dfrac{\omega_p^{\,2}\tau^2}{1+\omega^2\tau^2}\right) \\ \varepsilon_2 = 2n_f k_f = \varepsilon \dfrac{\omega_p^{\,2}\tau}{\omega\left(1+\omega^2\tau^2\right)} \end{cases}$$

Plasma frequency

$$\omega_p^{\,2} = \frac{nq^2}{\varepsilon m^*}$$

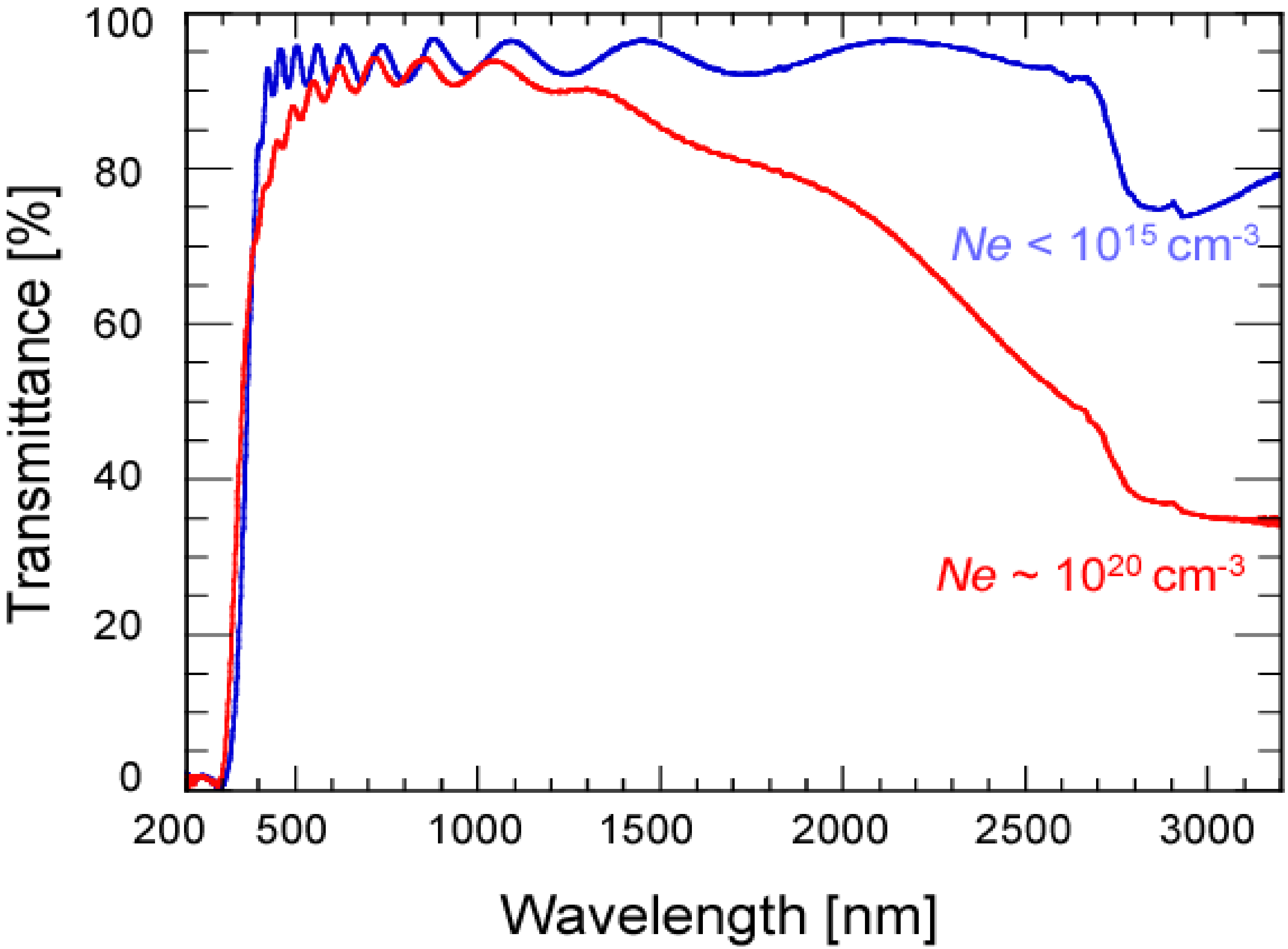
Optical conductivity

$$\sigma(\omega) = \omega\varepsilon_2(\omega) = \varepsilon\frac{\omega_p^{\,2}\tau}{1+\omega^2\tau^2}$$

物質	σ(10^5S/cm)	n (10^{22}cm^{-3})	μ(cm^2/Vs)	λ_p (nm)
Li	1.07	3.67	18.2	174
Ag	6.21	6.9	56	130
ITO	~0.1	~0.1	~100	~1000

E.g. for ITO, IR reflectivity (~800 nm) sharply increases when $n > 2\times10^{21}$cm^{-3}

Free carrier absorption



What are known from FCA

$$\varepsilon_1 = \varepsilon\left(1 - \frac{\omega_p^{\ 2}\tau^2}{1+\omega^2\tau^2}\right) \qquad \varepsilon_2 = \varepsilon\frac{\omega_p^{\ 2}\tau}{\omega\left(1+\omega^2\tau^2\right)}$$

Plasma freq. $\omega_p^{\ 2} = \dfrac{ne^2}{\varepsilon m^*}$ **Optical cond.** $\sigma(0) = \varepsilon\omega_p^{\ 2}\tau$

$$(= en\mu)$$

Known from experiments: ω_p, τ

Unknown: m*, n, τ

E.g., from Hall effect: $n_{FCA} \sim n_{Hall}$

=> Determine m*, τ => Optical mobility $\mu_{FCA} = \dfrac{e\tau}{m^*}$

E.g., employ single-crystal m*

=> determine n_{FCA}, τ => Difference of optical mobilities and n_{Hall} can be discussed

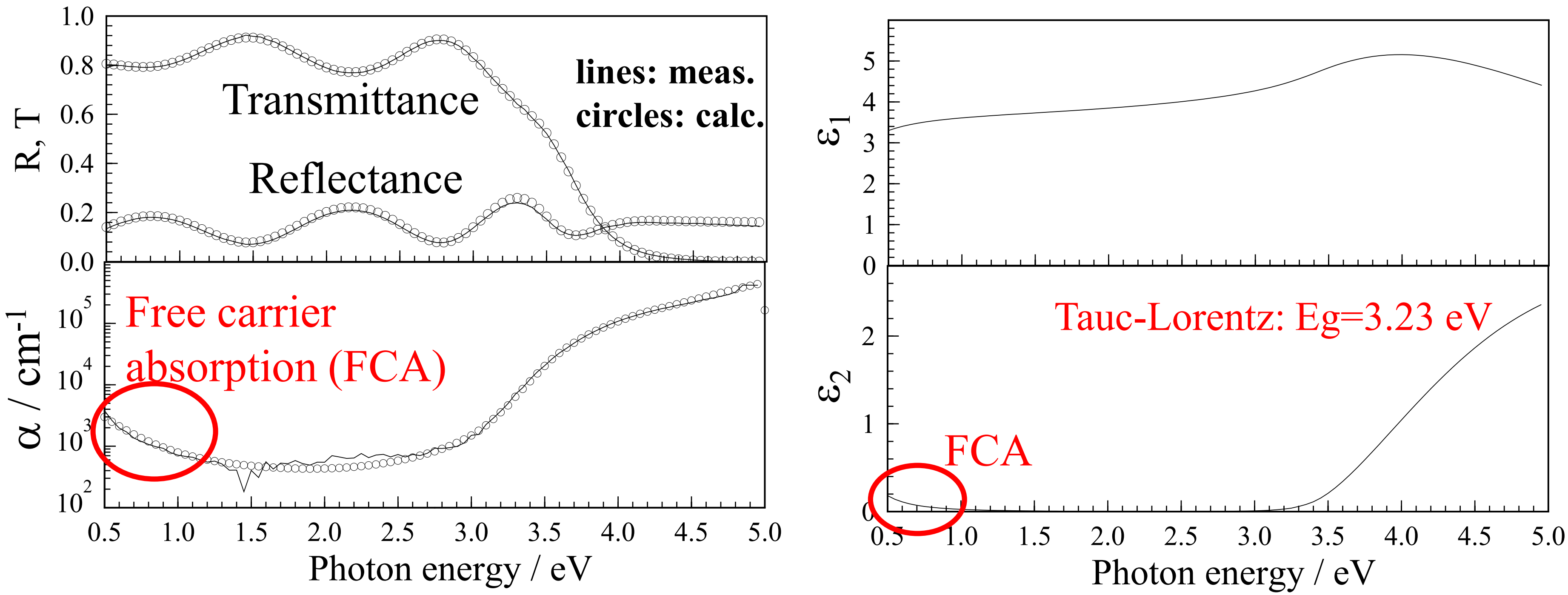
FCA analysis: a-IGZO

annealed HQ

T&R spectra combined + Film / Substrate layers optical model

Tauc-Lorentz model + Lorentz model (at ~E_G) + Drude model

Accuracy ~ 2% => $\alpha = -\ln(0.98)/d$ ~ 900 cm^{-1} (for d = 230 nm)



Band edge reproduced by a Tauc-Lorentz model

FCA fit well to a Drude model with a single τ:

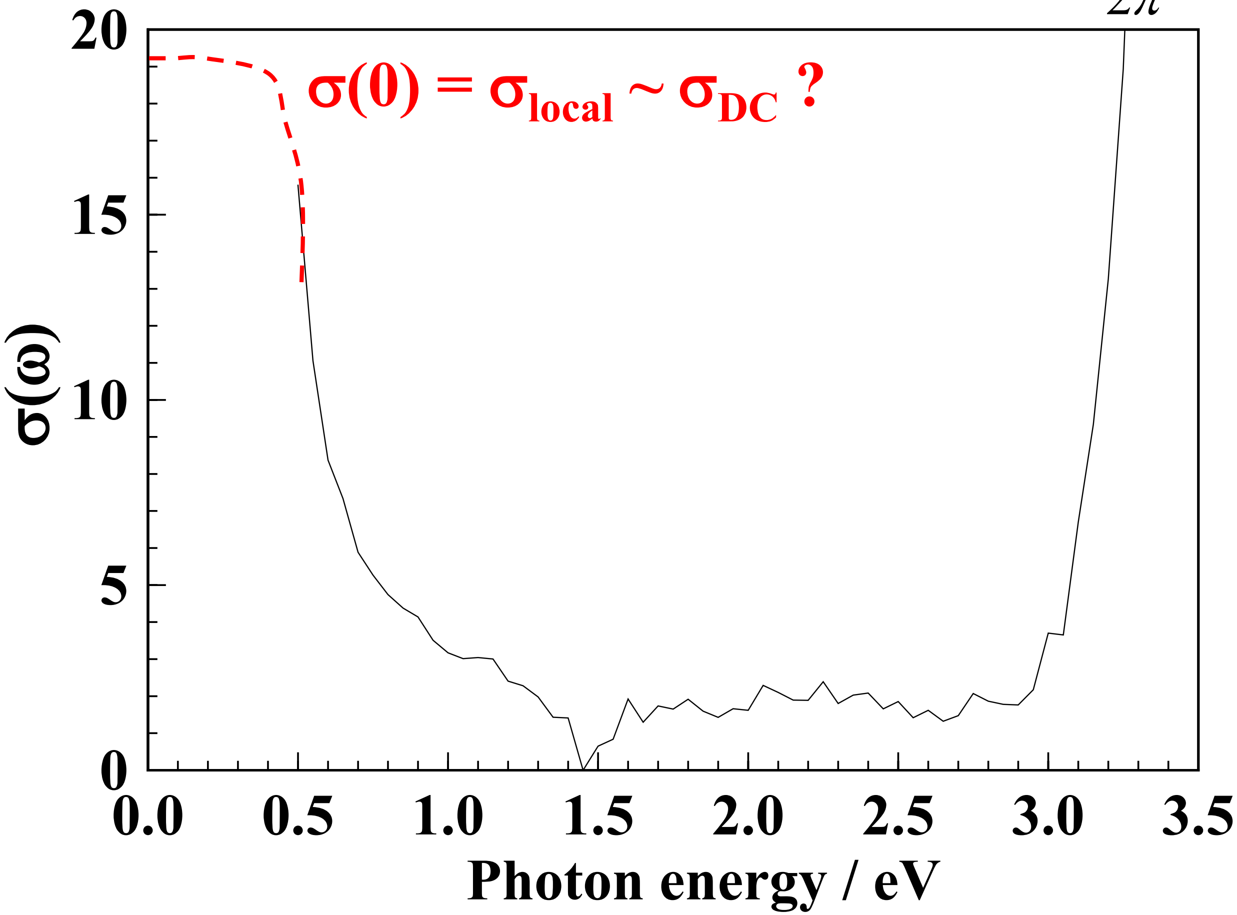
Free electron-like transport

Optical conductivity

annealed HQ a-IGZO

$$\sigma(\omega) = \omega\varepsilon_2(\omega) = \varepsilon \frac{\omega_p{}^2\tau}{1+\omega^2\tau^2}$$

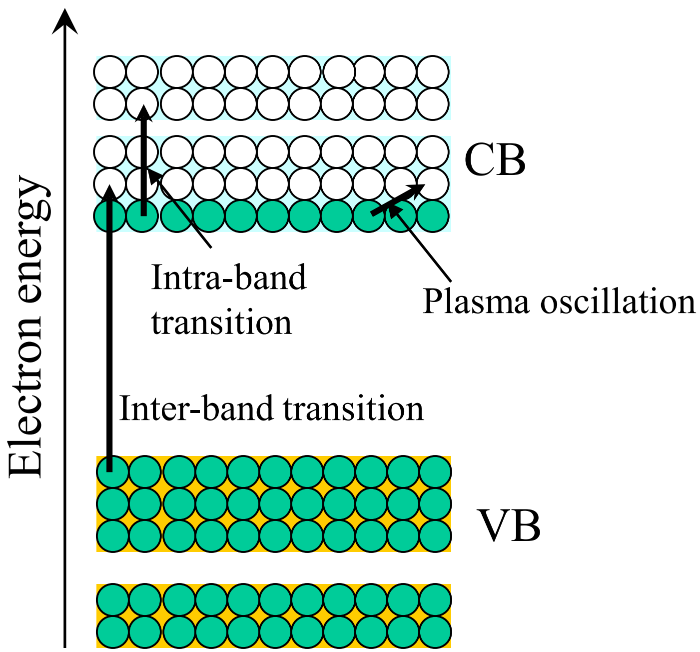
$$\varepsilon_2(\omega)/\,\varepsilon_0 = \frac{\lambda n}{2\pi}\alpha(\omega) = \frac{cn}{\omega}\alpha(\omega)$$

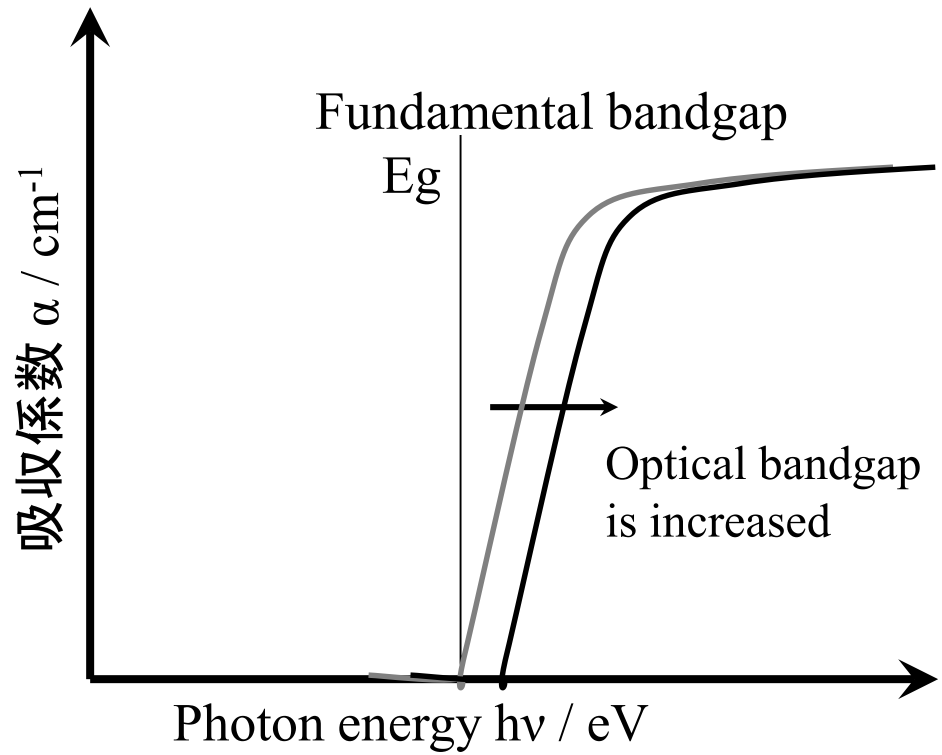


Can judge conductor or not even for powder materials

Optical bandgap for highly-doped semi.

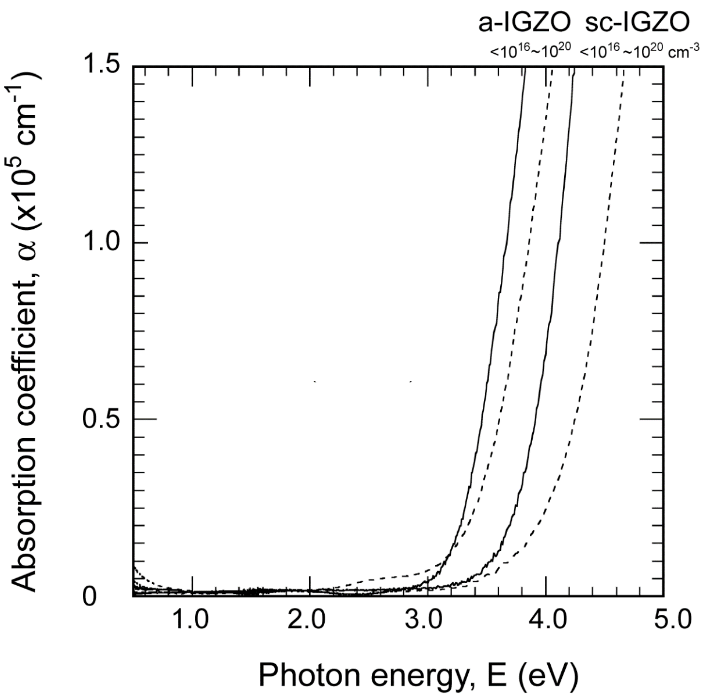
Band filling effect（Burstein-Moss shift)

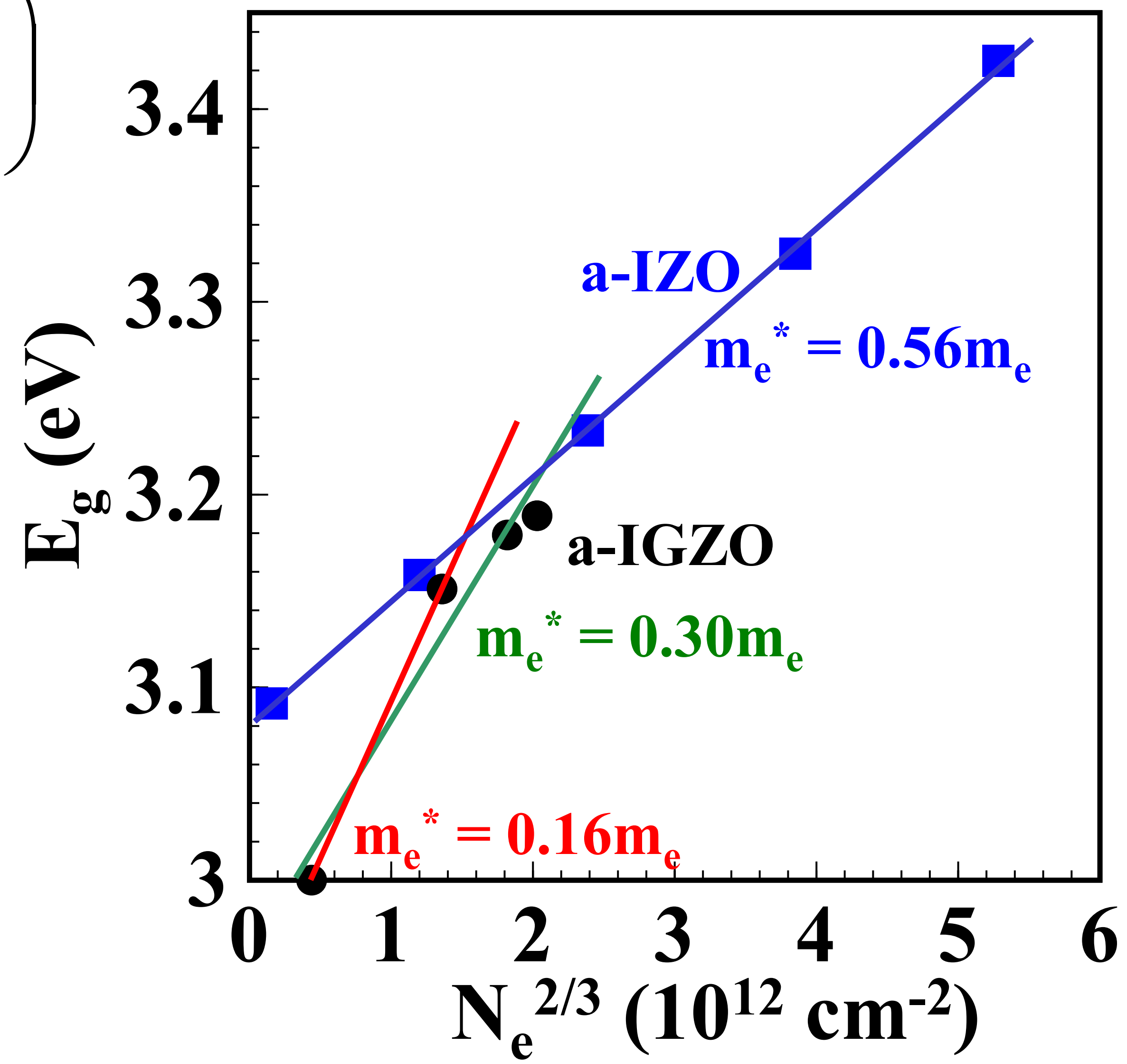




Band filling (BM shift)

$$\Delta E_g^{BM} = \frac{h^2}{m_{de}}\left(\frac{3N_e}{16\sqrt{2}\pi}\right)^{2/3}$$





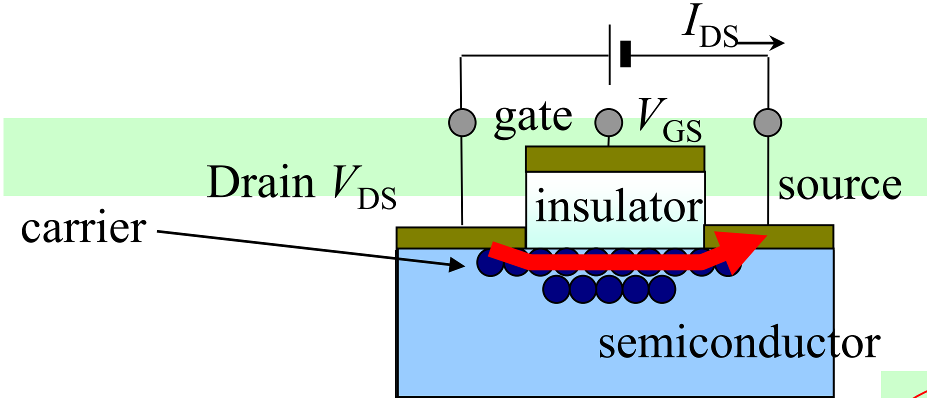
Field-effect mobility

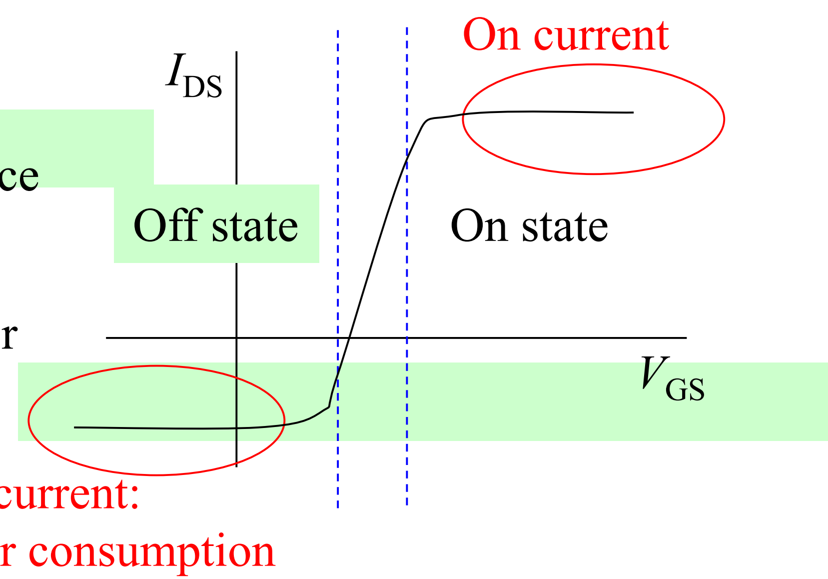
電界効果移動度

Operation of field-effect transistor (FET)

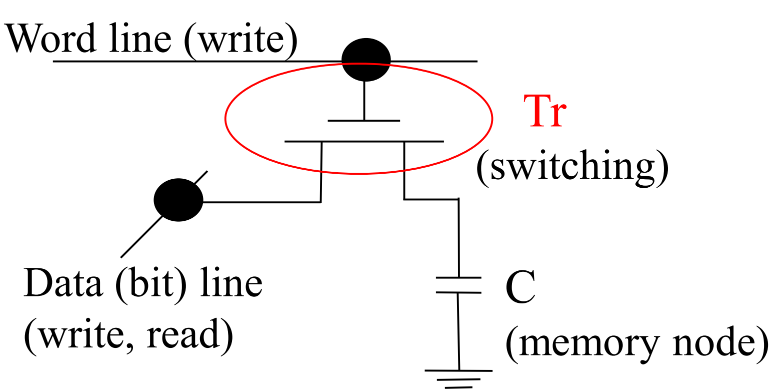
Two representative functions of transistor

1. **Amplification** **Use linear region ($I_{DS} \propto V_{GS}$)**
2. **Switching** **Use large on/off current ratio**





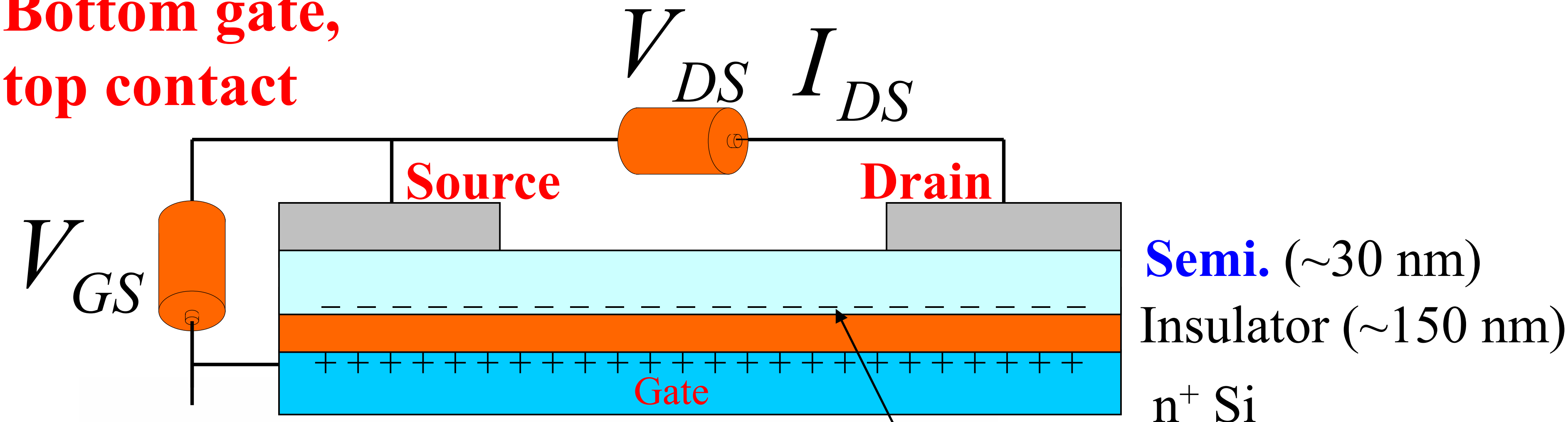
1C-1Tr memory



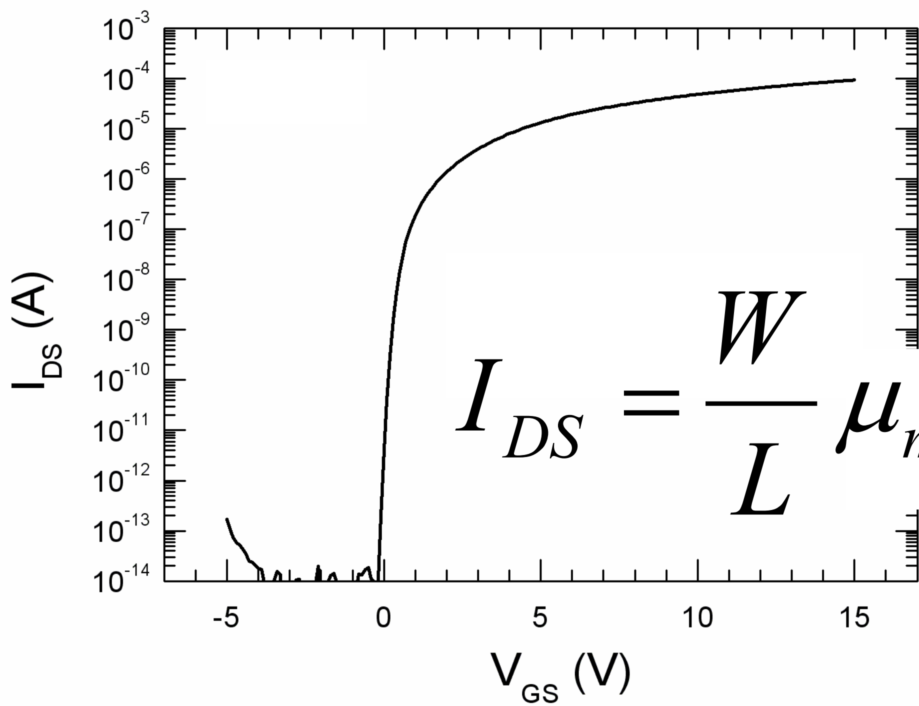
At V_{GS} = 0V
On state: Normally-on
Depletion-type
Off state: Normally-off
Enhancement-type

TFT structure and operation

Bottom gate, top contact



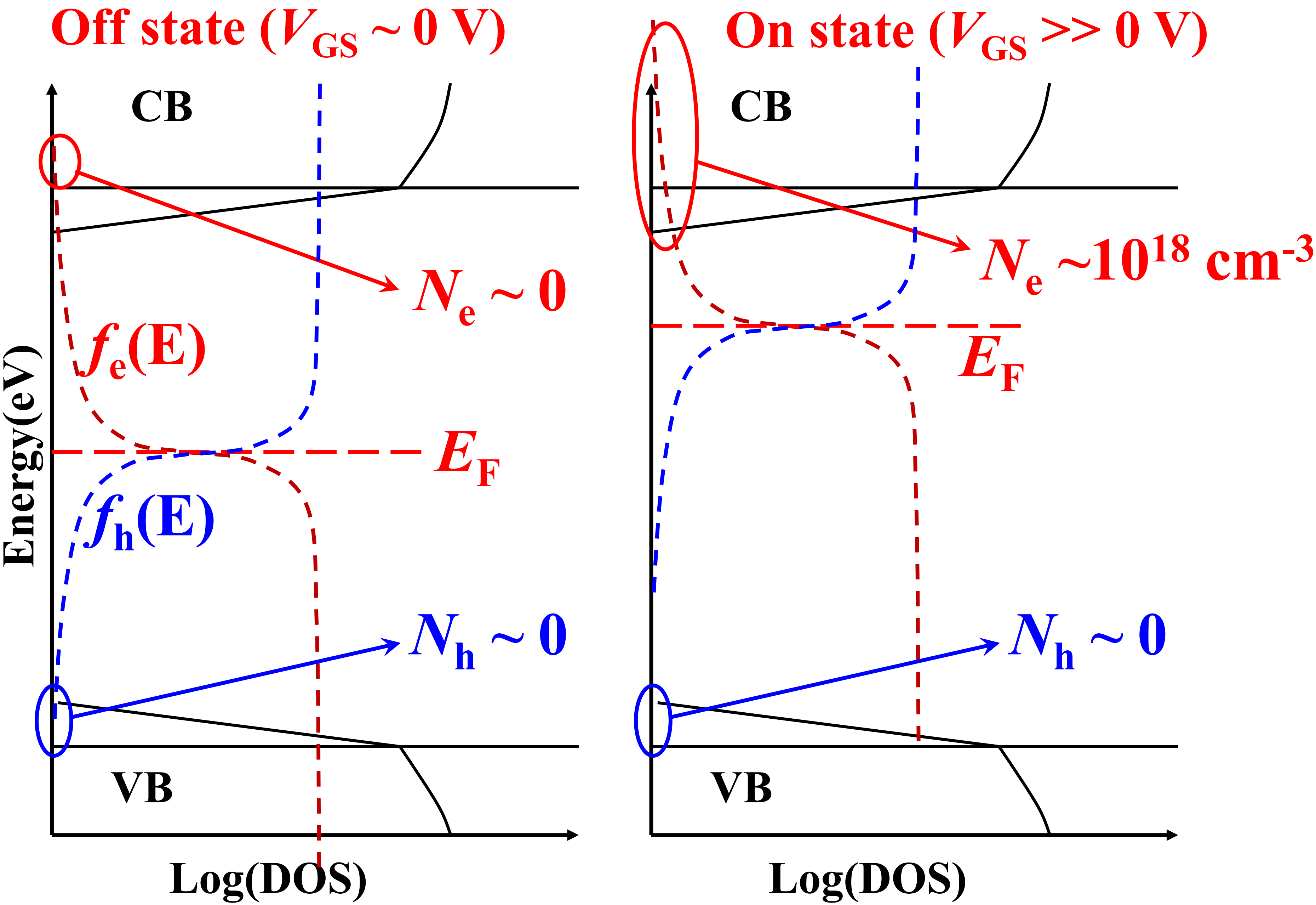
$$Q_{ind} \approx C_g (V_{GS} - V_{th})$$



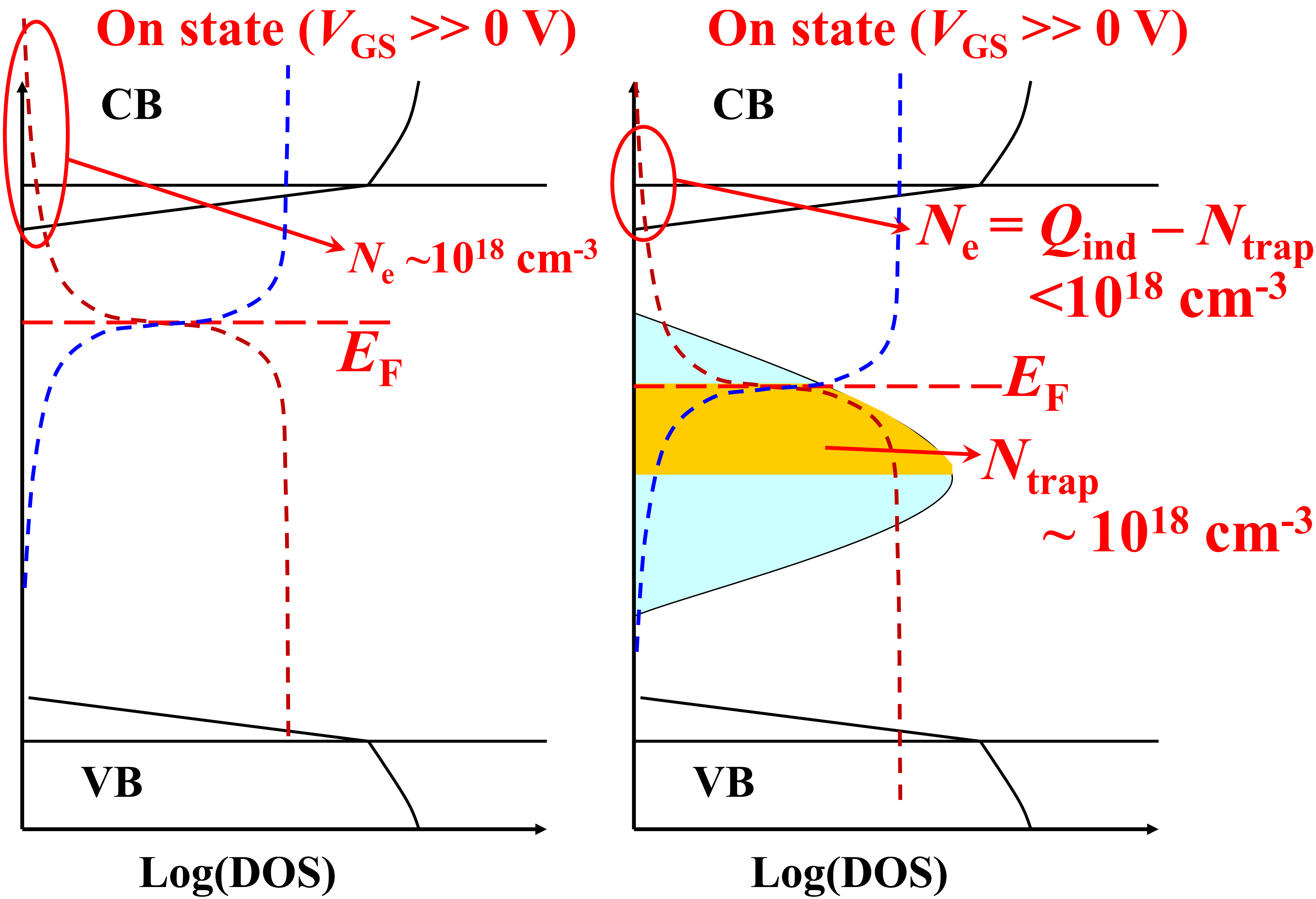
$$I_{DS} = \frac{W}{L} \mu_{mobile} C_g (V_{GS} - V_{th}) V_{DS}$$

Ideal case

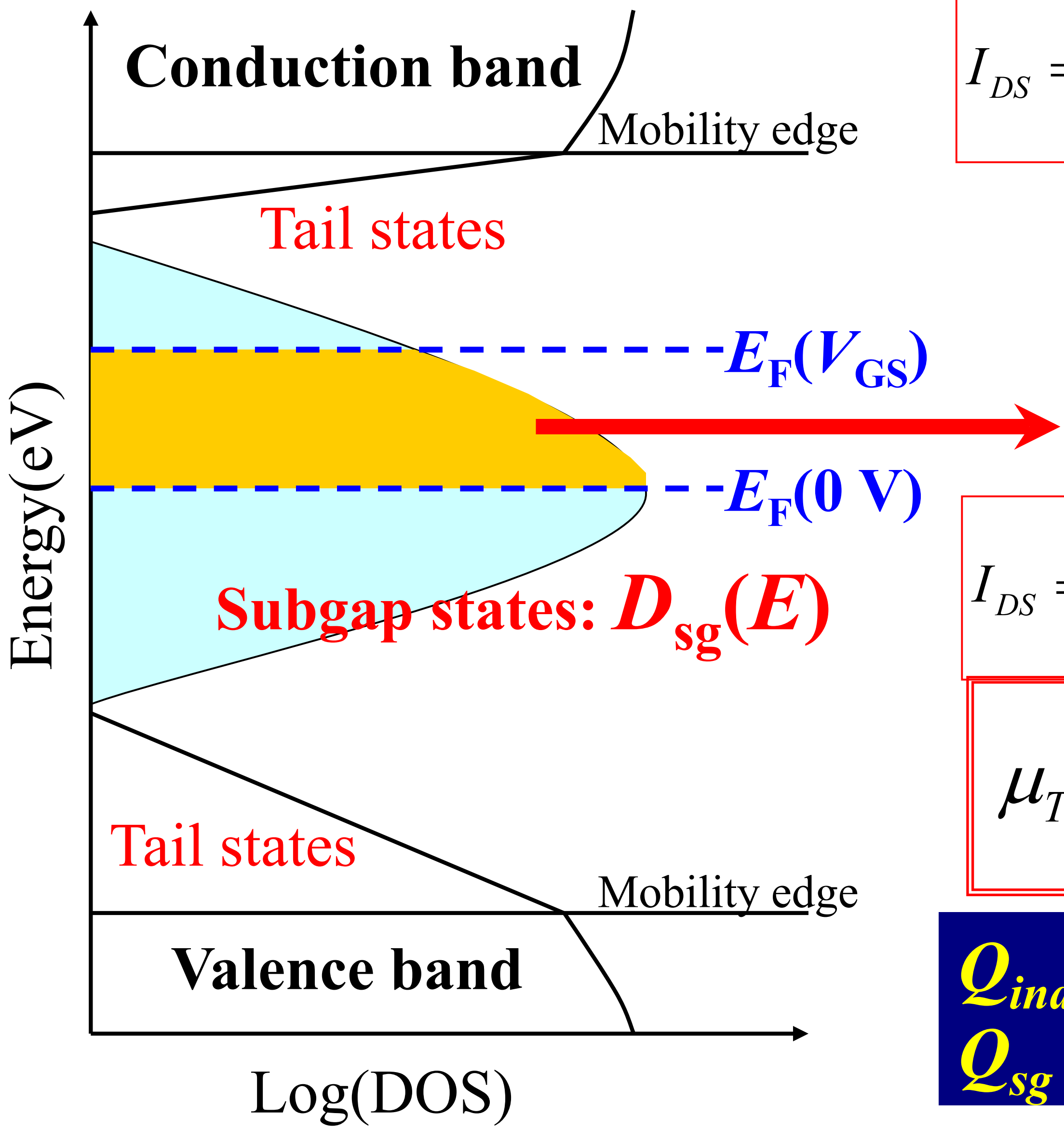
N-channel operation of TFT



Fermi level pinning by subgap traps



Effect of subgap states (trap states in E_g)



$$I_{DS} = \frac{W}{L}\mu_{drift}C_g\left[(V_{GS}-V_{th})V_{DS}-\frac{V_{DS}^2}{2}\right]$$

$$Q_{ind} \approx C_g V_{GS}$$

$$Q_{sg} = \int_{E_F(0)}^{E_F(V_{GS})} D_{sg}(E)\,dE$$

$$I_{DS} = \frac{W}{L}\mu_{TFT}C_g\left[(V_{GS}-V_{th})V_{DS}-\frac{V_{DS}^2}{2}\right]$$

$$\mu_{TFT} = \mu_{drift}\frac{Q_{ind}-Q_{sg}}{Q_{ind}}$$

$Q_{ind} \sim 10^{18}\ cm^{-3}$ (100ppm)
Q_{sg} must be $\ll Q_{ind}$

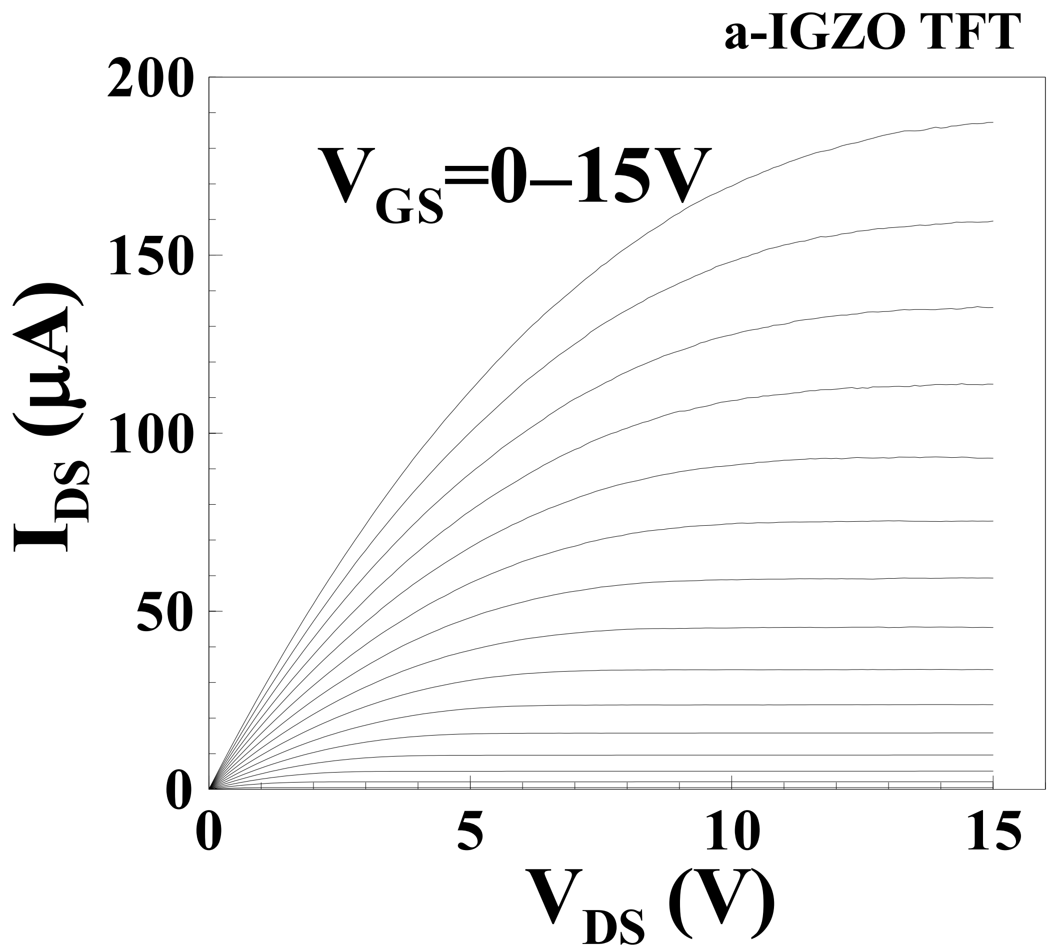
How to get high-performance TFT?

$$I_{DS} = \frac{W}{L}\mu_{drift}C_g\left[(V_{GS} - V_{th})V_{DS} - \frac{V_{DS}^2}{2}\right]$$

To obtain high I_{DS}

- Large W/L ratio
- Large C_g
- High V
- **Large μ_{drift} (Drift mobility)**

$$\sigma = en\mu_{drift}$$



Device simulation: TFT and drift mobilities

*Hsieh et al., APL **92**,133503 (2008)*

a-In-Ga-Zn-O TFT

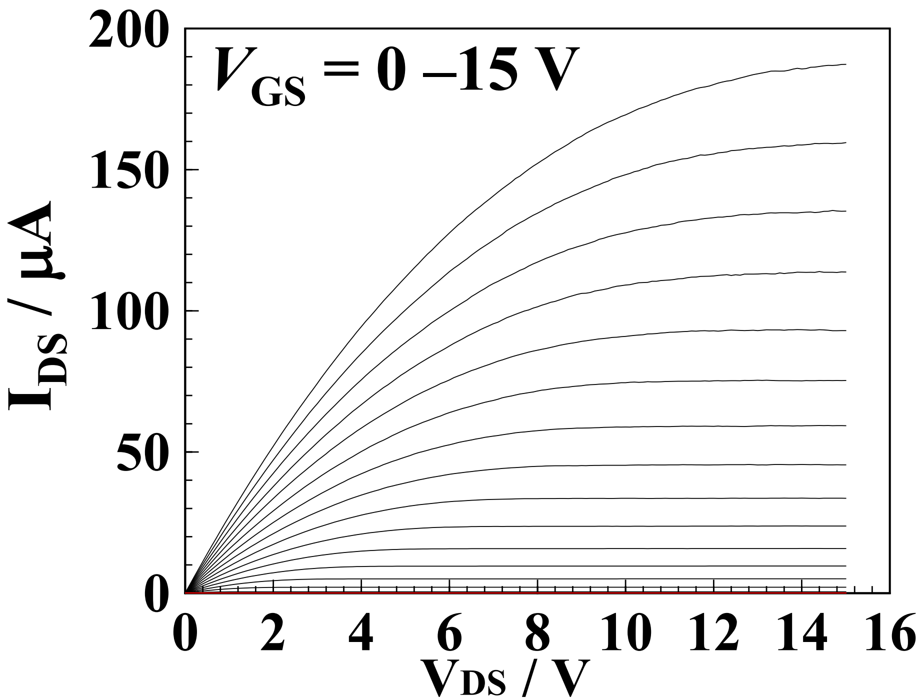
From Hall ($N_{e,Hall}$) & TFT (μ_{sat}) characteristics

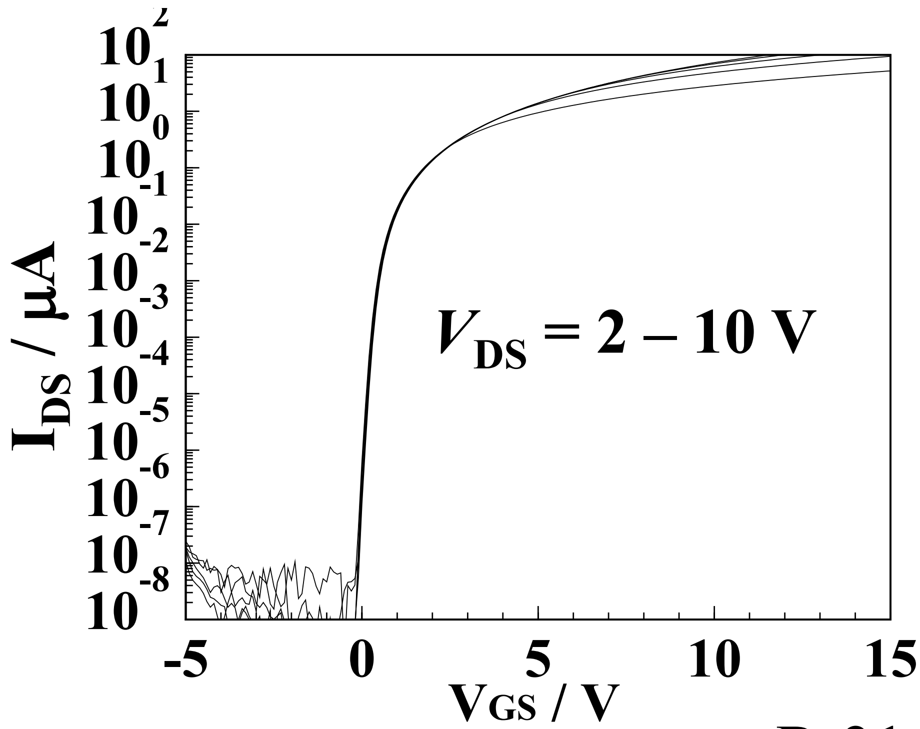
$N_{e,Hall}$ (cm^{-3})	μ_{sat} (cm^2/Vs)	V_{th} (V)
$\sim 1\times10^{15}$	**7.84**	4.9

From device simulation (drift mobility)

n_0 (cm^{-3})	μ_{drift} (cm^2/Vs)
1×10^{15}	**8.57**

12% of induced charges are trapped



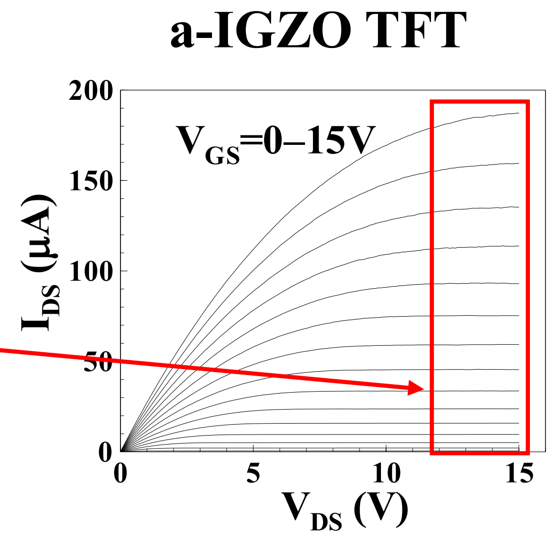


TFT characteristics: Saturation regime

$$I_{DS} = \frac{W}{L}\mu C_{OX}\left[(V_{GS} - V_{th})V_{DS} - \frac{{V_{DS}}^2}{2}\right]$$

$V_{DS} > V_p = V_{GS} - V_{th}$

$$I_{DS} = \frac{W}{2L}\mu C_{OX}(V_{GS} - V_{th})^2$$

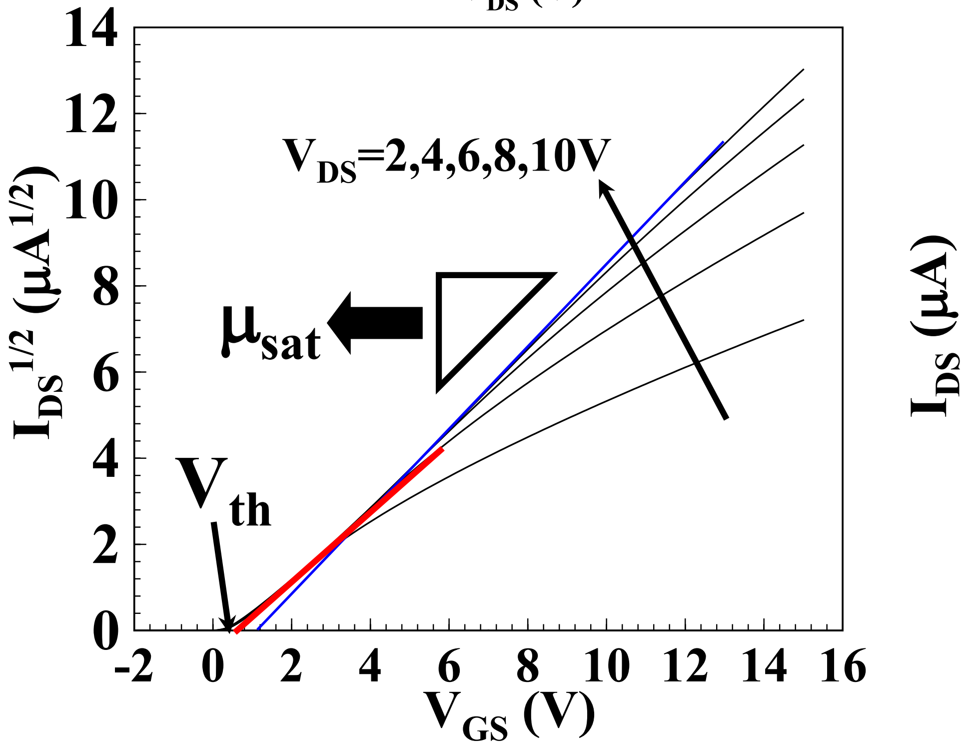


$${I_{DS}}^{1/2} = \sqrt{\frac{W}{2L}\mu C_{OX}}(V_{GS} - V_{th})$$

${I_{DS}}^{1/2}$ vs. V_{GS} plot

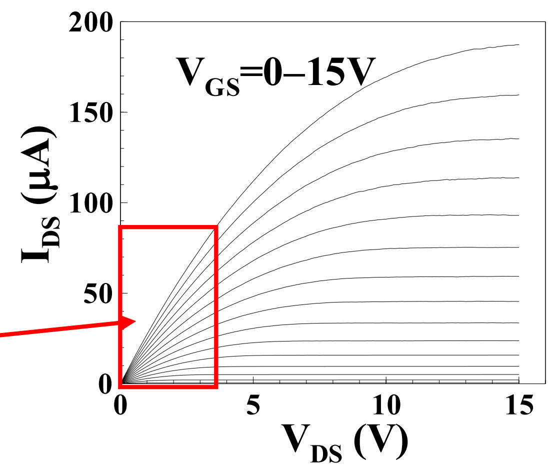
V_{GS}-axis cross-section: V_{th}

Slope: Saturation mobility, μ_{sat}



TFT characteristics: Linear regime

$$I_{DS} = \frac{W}{L}\mu C_{OX}\left[(V_{GS} - V_{th})V_{DS} - \frac{V_{DS}{}^2}{2}\right]$$



V_{DS} << V_p (V_{GS}) (e.g., << 0.1 V)

$$I_{DS} = \frac{W}{L}\mu C_{OX}V_{DS}(V_{GS} - V_{th})$$

I_{DS} is proportional to V_{DS}:
- **I_{DS} vs. V_{GS} plot**
  - **V_{GS}-axis cross-section: V_{th}**
  - **Slope: Linear-regime field-effect mobility**

Effective mobility: μ_{eff}

$$\mu_{eff} = g_{DS}\frac{L}{WC_{OX}(V_{GS} - V_{th})}$$

$$g_{DS} = \frac{dI_{DS}}{dV_{DS}}$$ **Drain conductance**

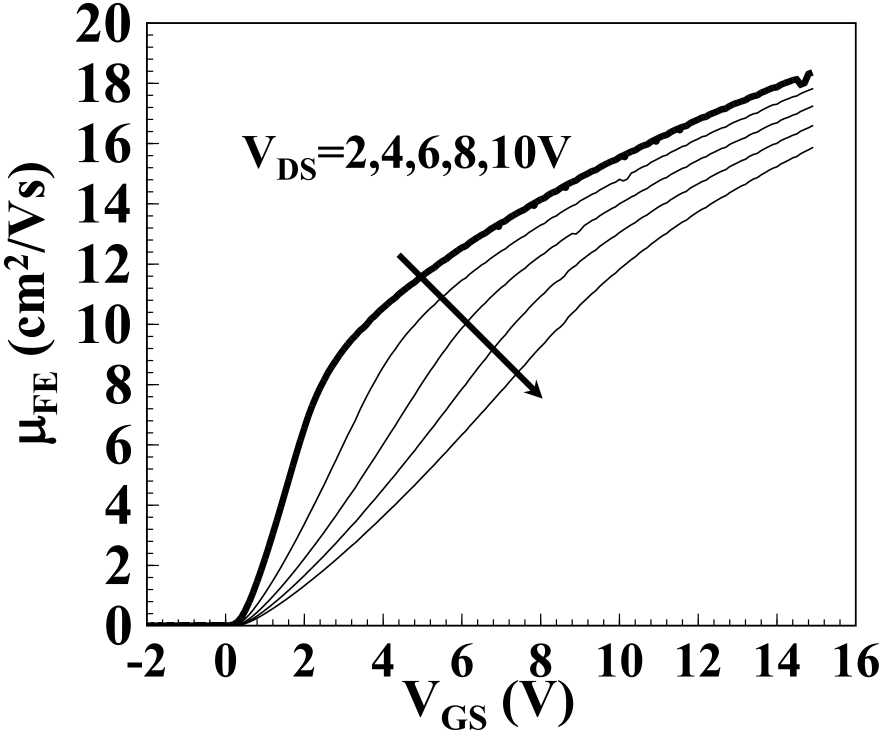
Field-effect mobility: μ_{FE}

$$\mu_{FE} = g_m\frac{L}{WC_{OX}V_{DS}}$$

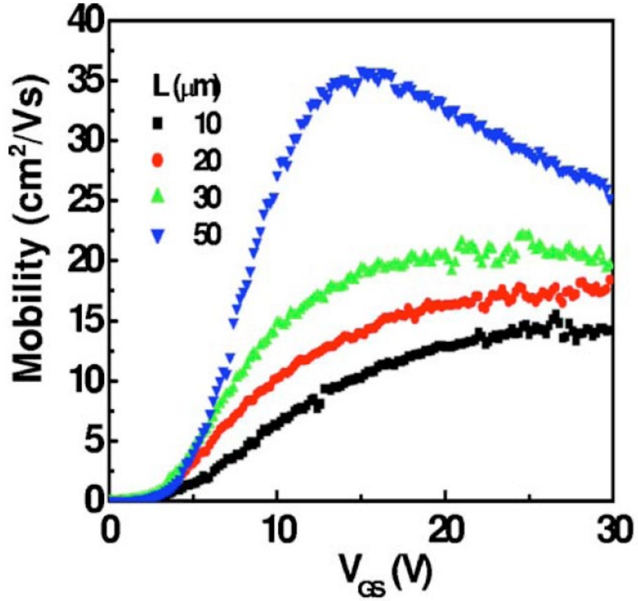
$$g_m = \frac{dI_{DS}}{dV_{GS}}$$ **Transconductance**

V_{GS} dependence of FE Mobility

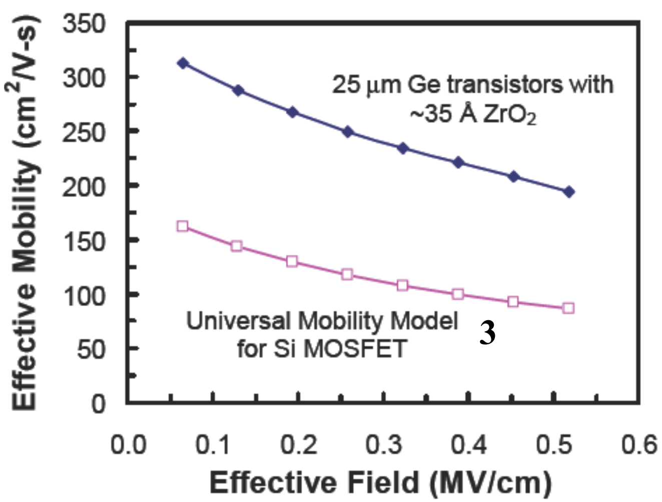
a-IGZO TFT / SiO_2/c-Si



a-IGZO TFT / SiO_2/MoW/glass [1]
etch-stopper inverted-staggered



MOSFET [2]



1. M.Kim et al., APL **90**, 212114 (2007)
2. C.O. Chui, H. Kim, D. Chi, B.B. Triplett, P.C. McIntyre, K.C. Saraswat, IEDM (2002) p.437
3. K. Chen, H. C. Wann, P. K. Ko, and C. Hu, IEEE Electr. Dev. Lett., **17**, 202 (1996)

Space charge limited current (SCLC)

空間電荷制限電流

Thermiomic emission of e^- to vacuum: Space-charge limited current (SCLC)

「荷電粒子ビーム工学」, コロナ社

Electrostatic potential is formed by the e^- emitted to vacuum

Electron velocity $v(x)$, electrostatic potential $V(x)$ are functions of x

$$\frac{1}{2}mv(x)^2 = eV$$

Current continuity $j(x) = en(x)v(x) = j$

Poisson equation $$\frac{d^2V(x)}{dx^2} = \frac{en_e(x)}{\varepsilon_0} = \frac{J}{\varepsilon_0}\left(\frac{m_e}{2eV}\right)^{1/2}$$

Multiply $\frac{dV}{dx}$ and integrate $$\left(\frac{dV(x)}{dx^2}\right)^{1/2} = \frac{4J}{\varepsilon_0}\left(\frac{m_e}{2e}\right)^{1/2} V^{1/2} + C$$

Maximum current is obtained by $E(0) = 0$

$$V = \left(\frac{3}{4}\right)^{4/3}\left(\frac{4J}{\varepsilon_0}\right)^{2/3}\left(\frac{m_e}{2e}\right)^{1/3} x^{4/3}$$

$$J = \frac{4\varepsilon_0}{9}\left(\frac{2e}{m_e}\right)^{1/2}\frac{V^{3/2}}{d^2}$$

Child-Langmuir equation

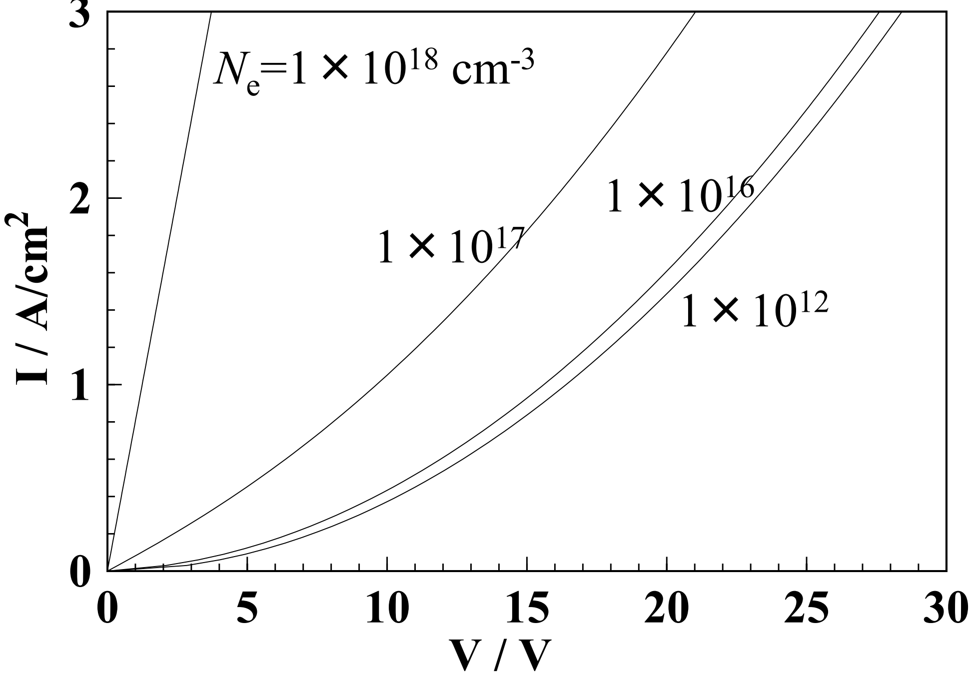
Ohm law is not valid anymore

SCLC vs Ohmic current

Ohmic current: $J = \sigma E$

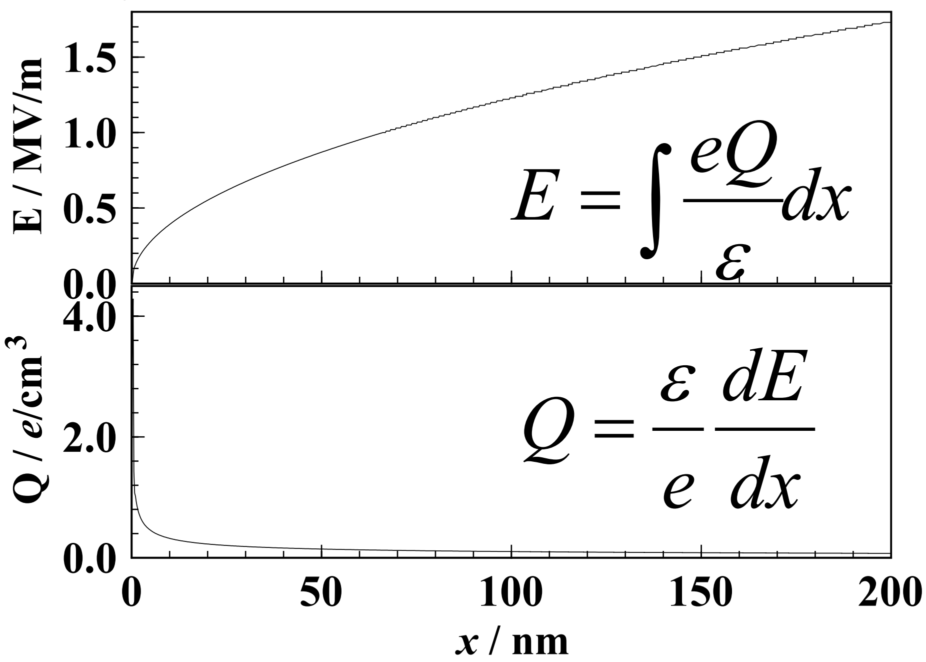
SCLC: $J = \frac{9}{8}\varepsilon\mu\frac{E^2}{d}$

$\varepsilon_r = 3.0\ \varepsilon_0$
$\mu_e = 1\times10^{-4}\ \mathrm{cm^2/Vs}$
$d = 200$ nm



$N_e = 1\times10^{12}\ \mathrm{cm^{-3}}$

$$\frac{d^2V}{dx^2} = \frac{\rho}{\varepsilon}$$



Ohmic vs. SCLC

Ohmic contact: $I = R^{-1} V$

SCLC with no trap state: $I = \frac{9}{8}\varepsilon\mu\frac{V^2}{d^3}$

SCLC with trap state: $h(E) = \frac{H_t}{E_t}\exp\left(-\frac{E}{E_t}\right)$

$$I = e^{1-l}\mu_p N_v \left(\frac{2l+1}{l+1}\right)^{l+1}\left(\frac{l}{l+1}\frac{\varepsilon}{H_t}\right)^{l}\frac{V^{l+1}}{d^{2l+1}}$$

$$l = T_c / T = E_t / k / T$$

V. Kumar, S.C. Jain, A.K. Kapoor, J. Poortmans, R. Mertens, *Trap density in conducting organic semiconductors determined from temperature dependence of J-V characteristics*, JAP **94** (2003) 1283.

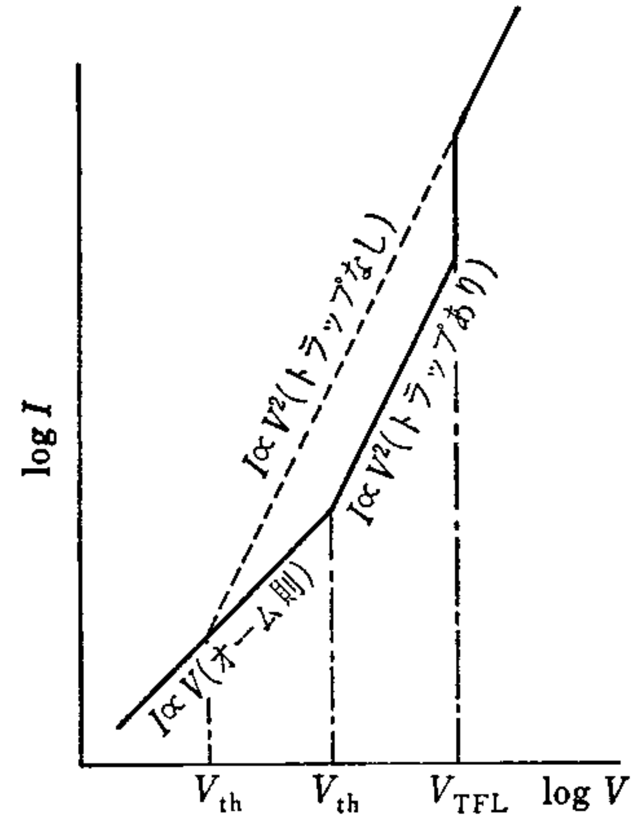
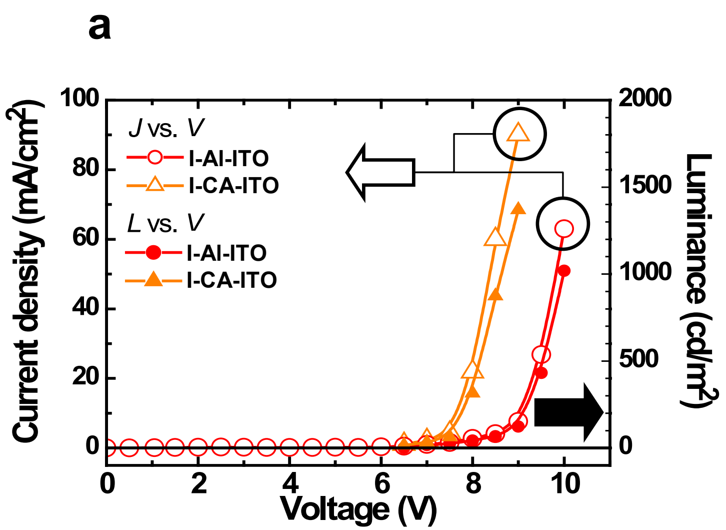
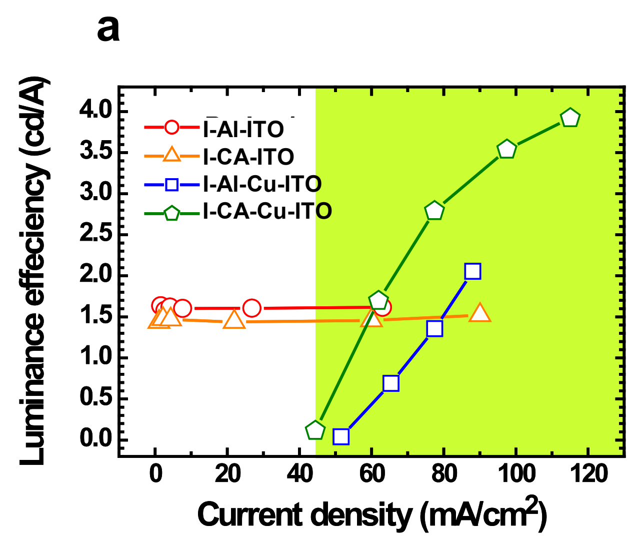


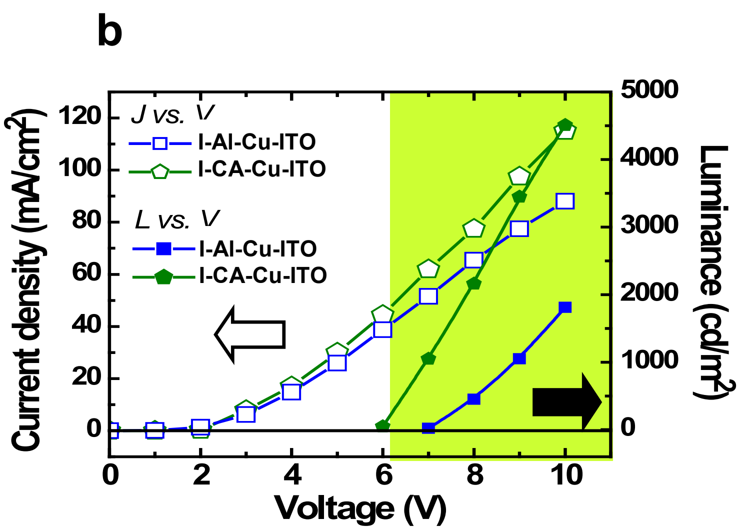
図 3.18 空間電荷制限電流

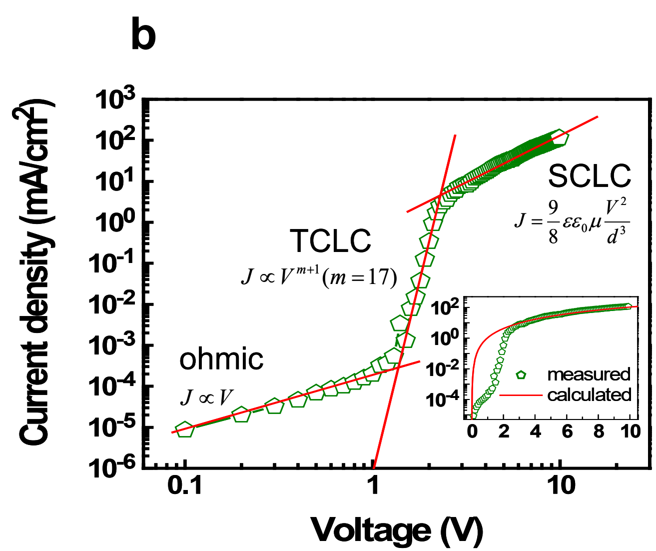
Ex. For C12A7e$^-$/Cu$_x$Se OLED

Yanagi et al., J. Phys. Chem. C 113 (2009) 18379









Different mobilities

- Drift mobility (definition)

  $\mu_d = E / v_{drift}$

  measured by time-of-flight methods

  Very thick film required

- Conductivity mobility

  $\mu_c = \sigma / (en)$: How to determine n?

- Hall mobility

  $V_H = R_H I_x B_Z / d$, $R_H = \gamma / en_{Hall}$

  $\mu_{Hall} = \sigma / (en_{Hall}) = \gamma\mu_d$

  ($\gamma = 1 - 2$: Hall factor, or scattering factor)

  DC mobility including grain boundary effects

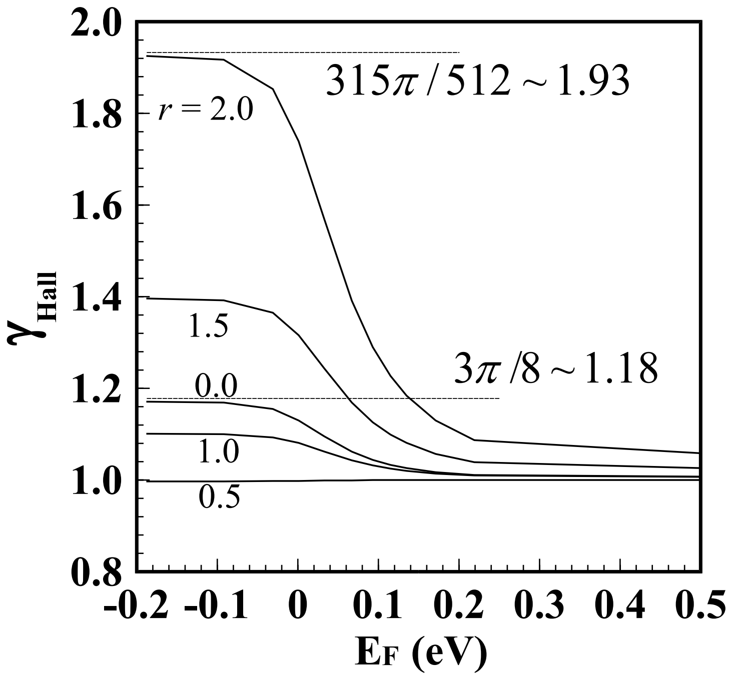
- Optical mobility

  From free carrier absorption

  High-doping required, Local mobility

- Field-effect mobility

  Largely depends on quality of TFT / FET

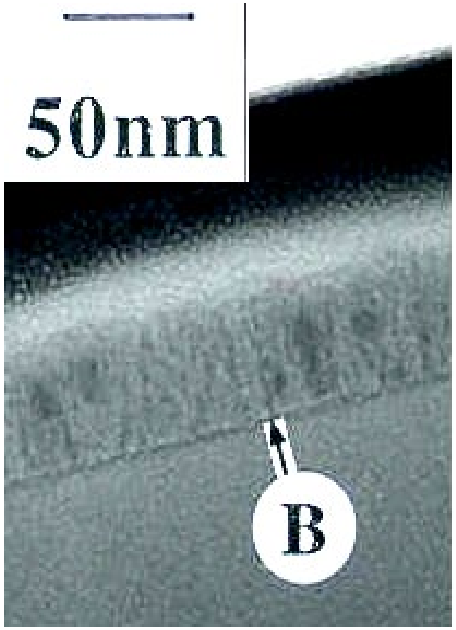


Electronic conduction in polycrystals

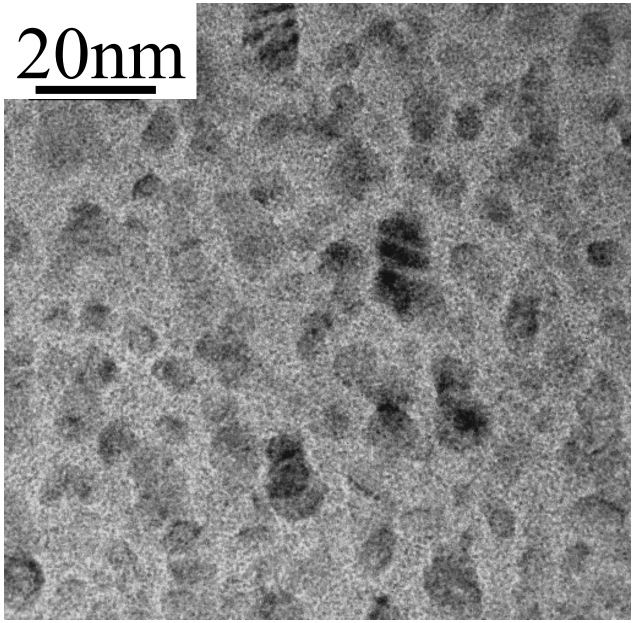
多結晶半導体の伝導

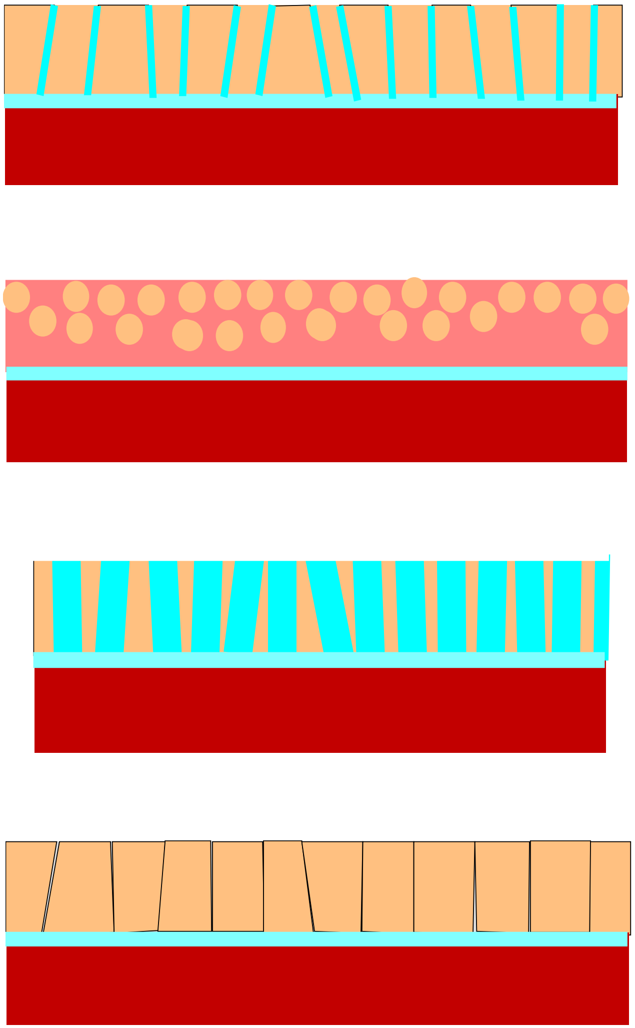
Microstructures of poly-Si

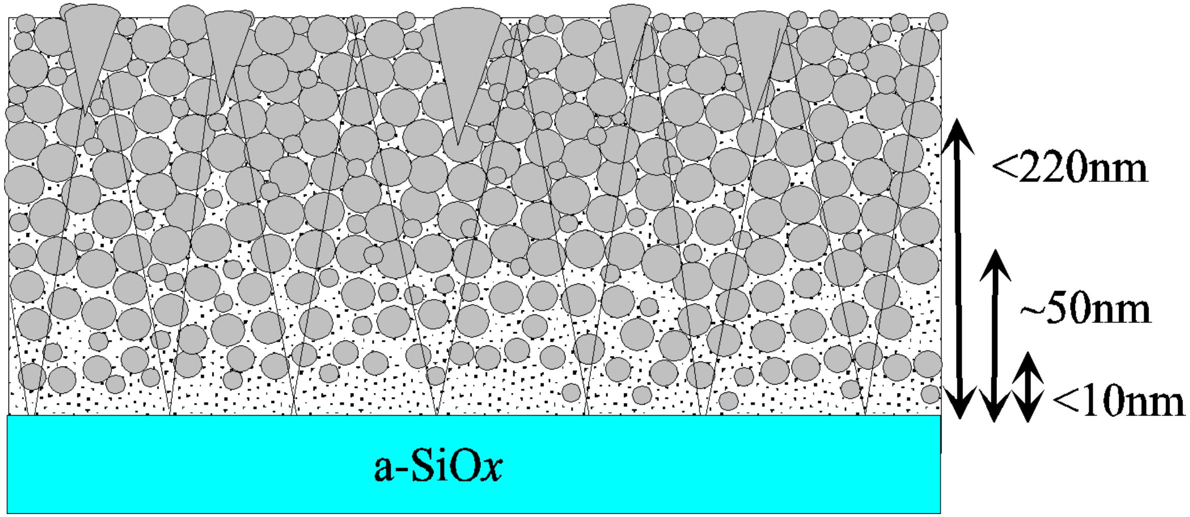
Cross-section



Plan view

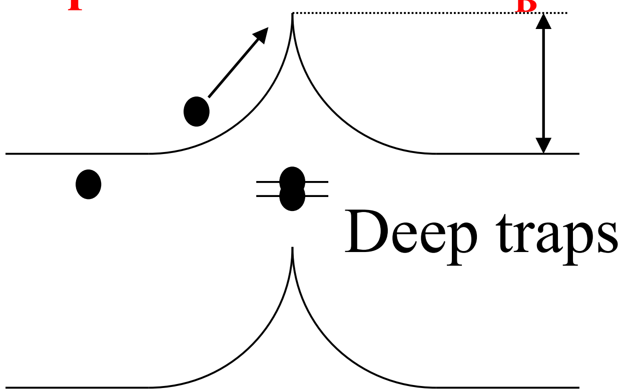






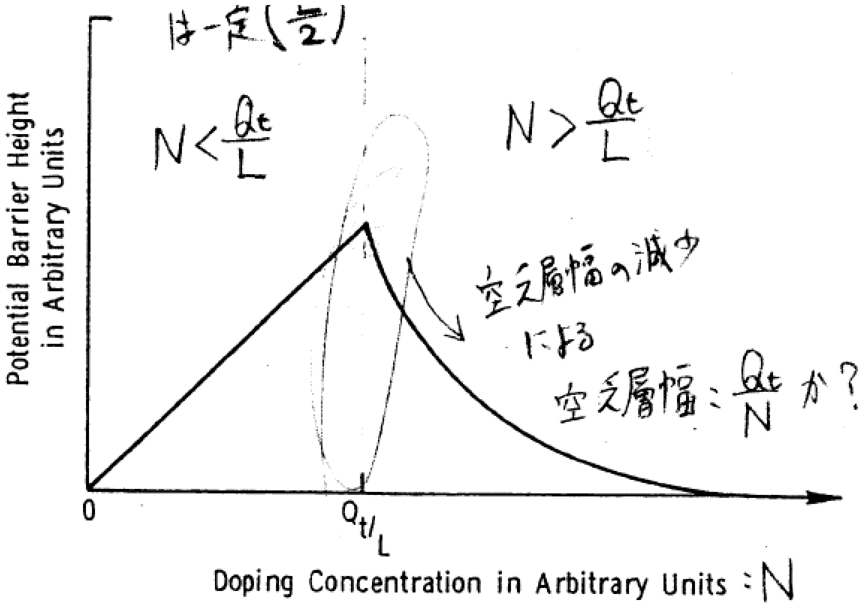
Theory for polycrystalline semi.: Seto model

GB potential barrier: V_B

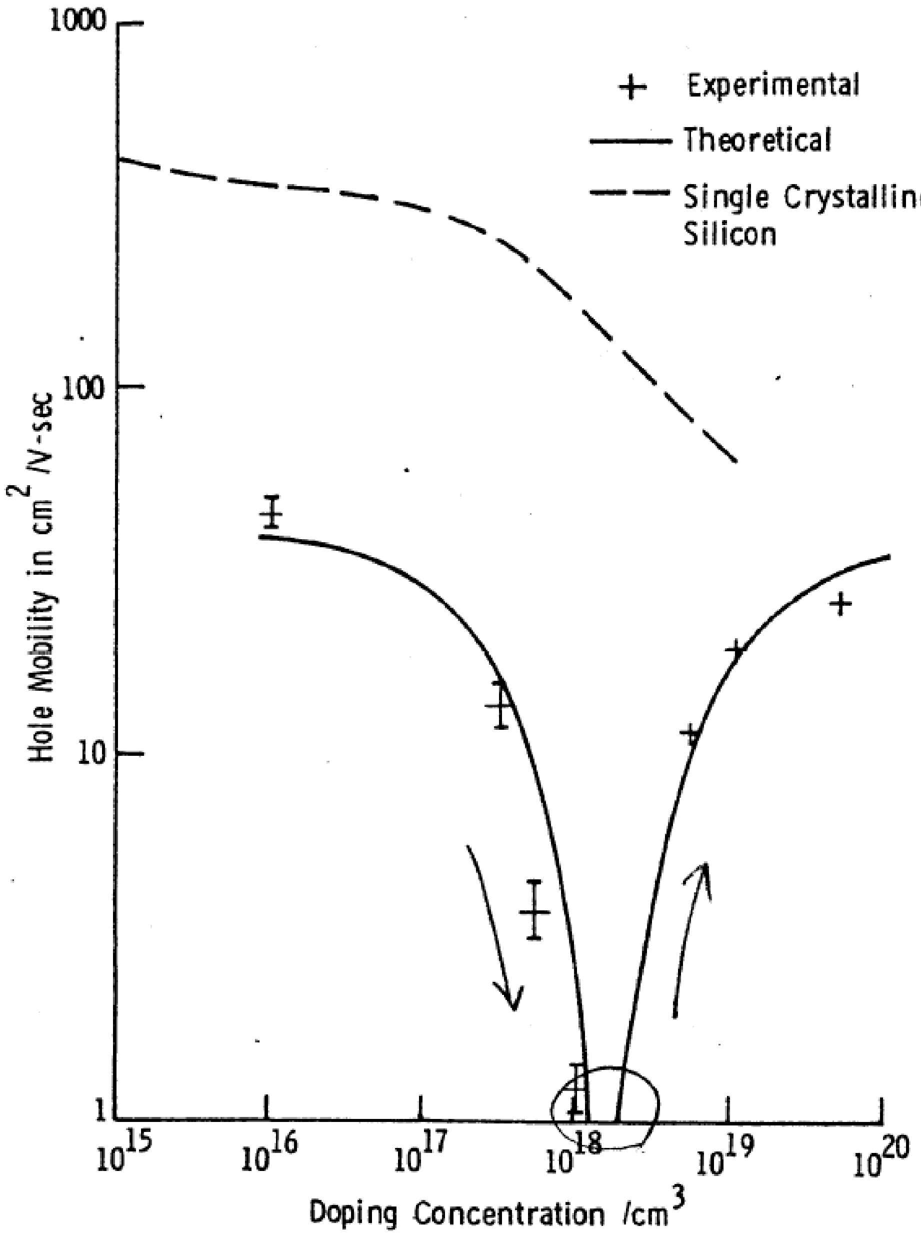


$$I(V) = 2qn_P\left(\frac{kT}{2\pi m^*}\right)^{1/2}\exp\left(-\frac{qV_B}{k_BT}\right)\sinh\left(-\frac{qV}{2nk_BT}\right)$$

$$\mu = Lq(1/2\pi m^* kT)^{1/2}\exp(-V_B/kT)$$

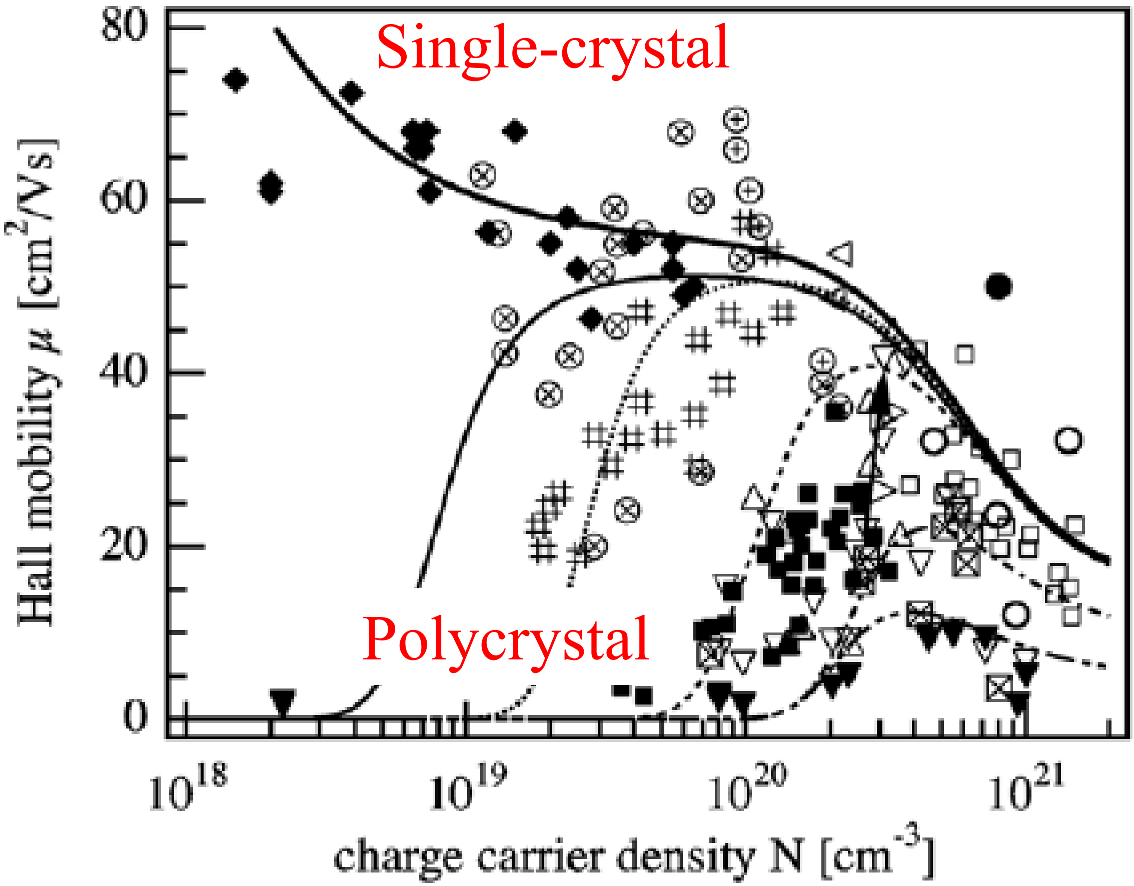


John Y.W. Seto, JAP 46 (1975) 5247

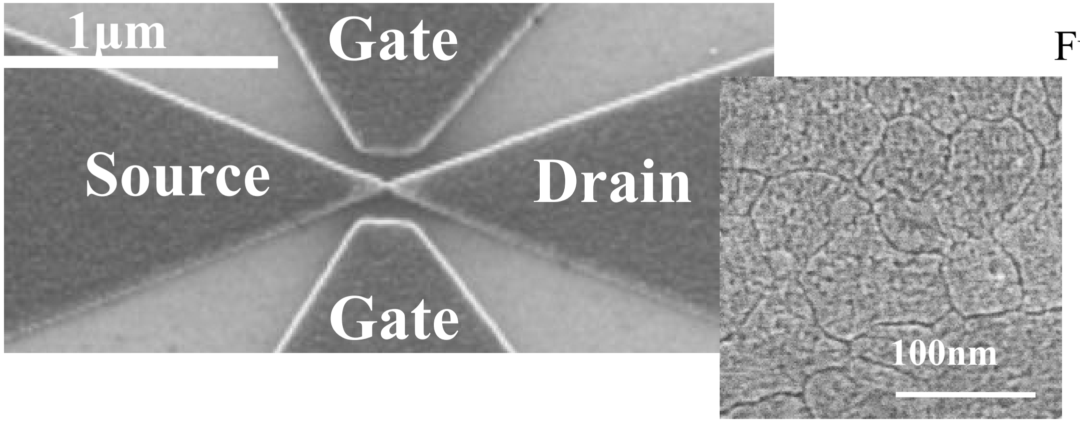


ZnO mobility

Ellmer et al., Thin Solid Films **516** (2008) 4620

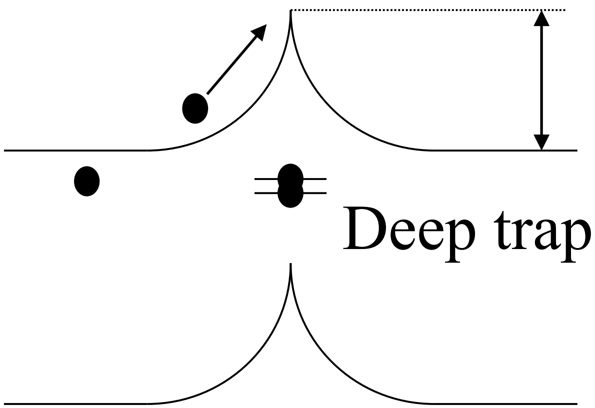


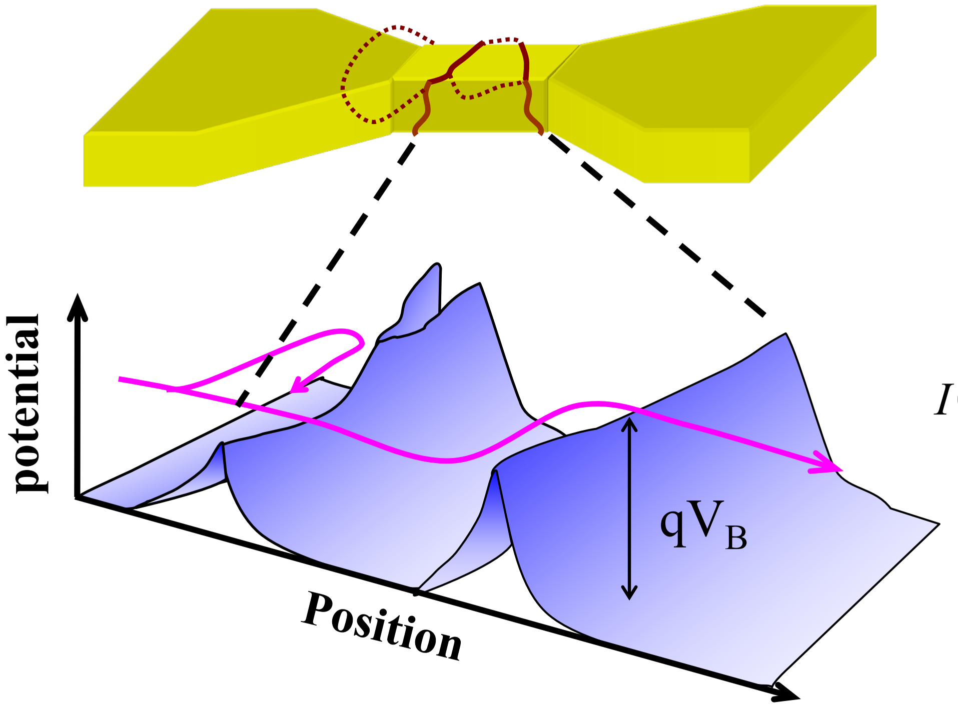
Measured using nanowire device



Furuta et al., Jpn. J. Appl. Phys. **40**, L615 (2001)

GB potential barrier: V_B





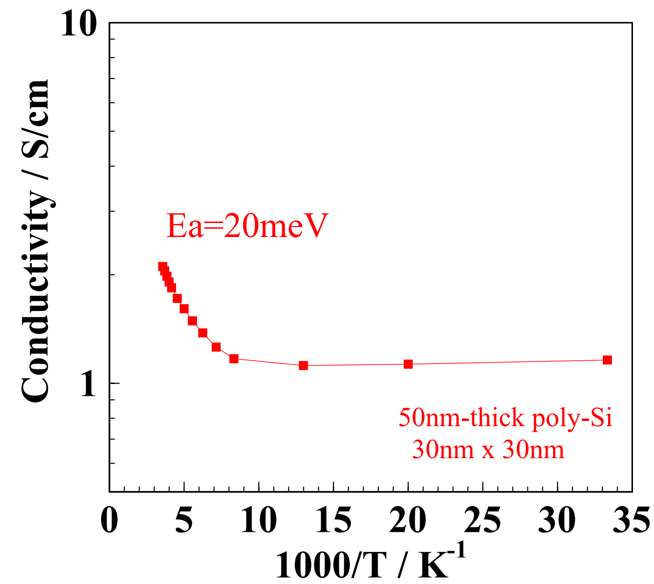
$$I(V) = 2qn_P\left(\frac{kT}{2\pi m^*}\right)^{1/2}\exp\left(-\frac{qV_B}{k_BT}\right)\sinh\left(-\frac{qV}{2nk_BT}\right)$$

$$\mu = Lq(1/2\pi m^* kT)^{1/2}\exp(-E_B/kT)$$

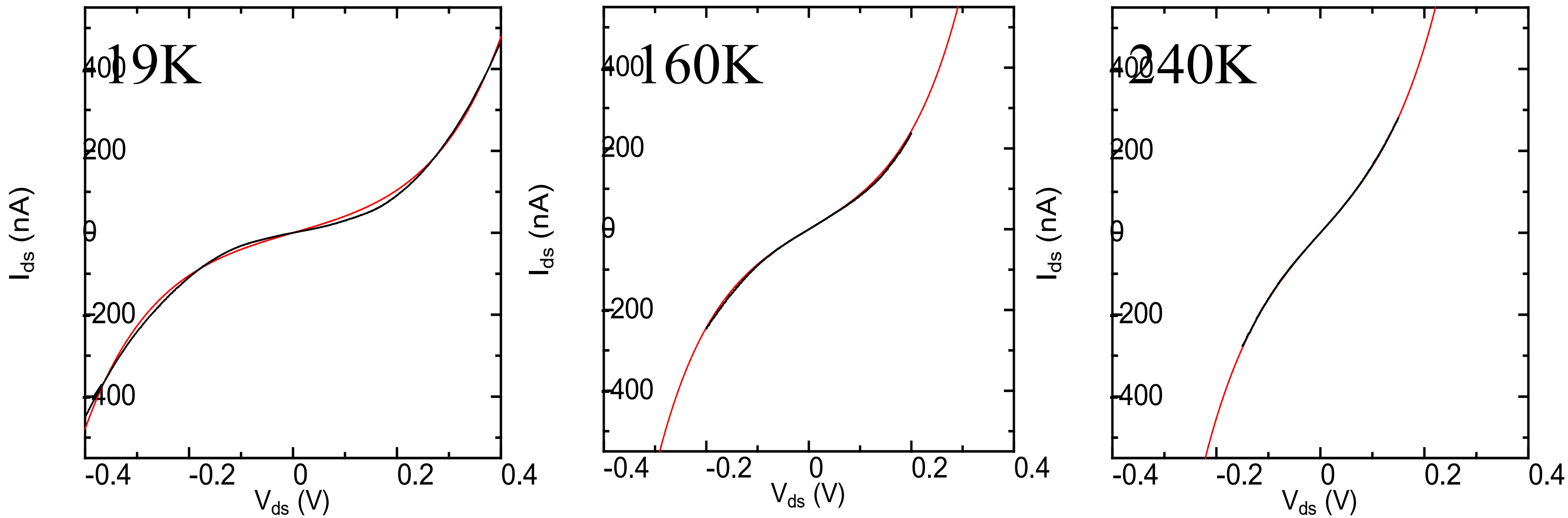
J.Y.W. Seto, *The electrical properties of polycrystalline silicon films*, J. Appl. Phys. 46 (1975) 5247.

Kamiya et al., MRS Proc. **664**, A16.2 (2001)

Double-Schottky barrier-controlled transport in poly-Si



$$I(V) = 2qn_P\left(\frac{kT}{2\pi m^*}\right)^{1/2}\exp\left(-\frac{qV_B}{k_BT}\right)\sinh\left(-\frac{qV}{2nk_BT}\right)$$

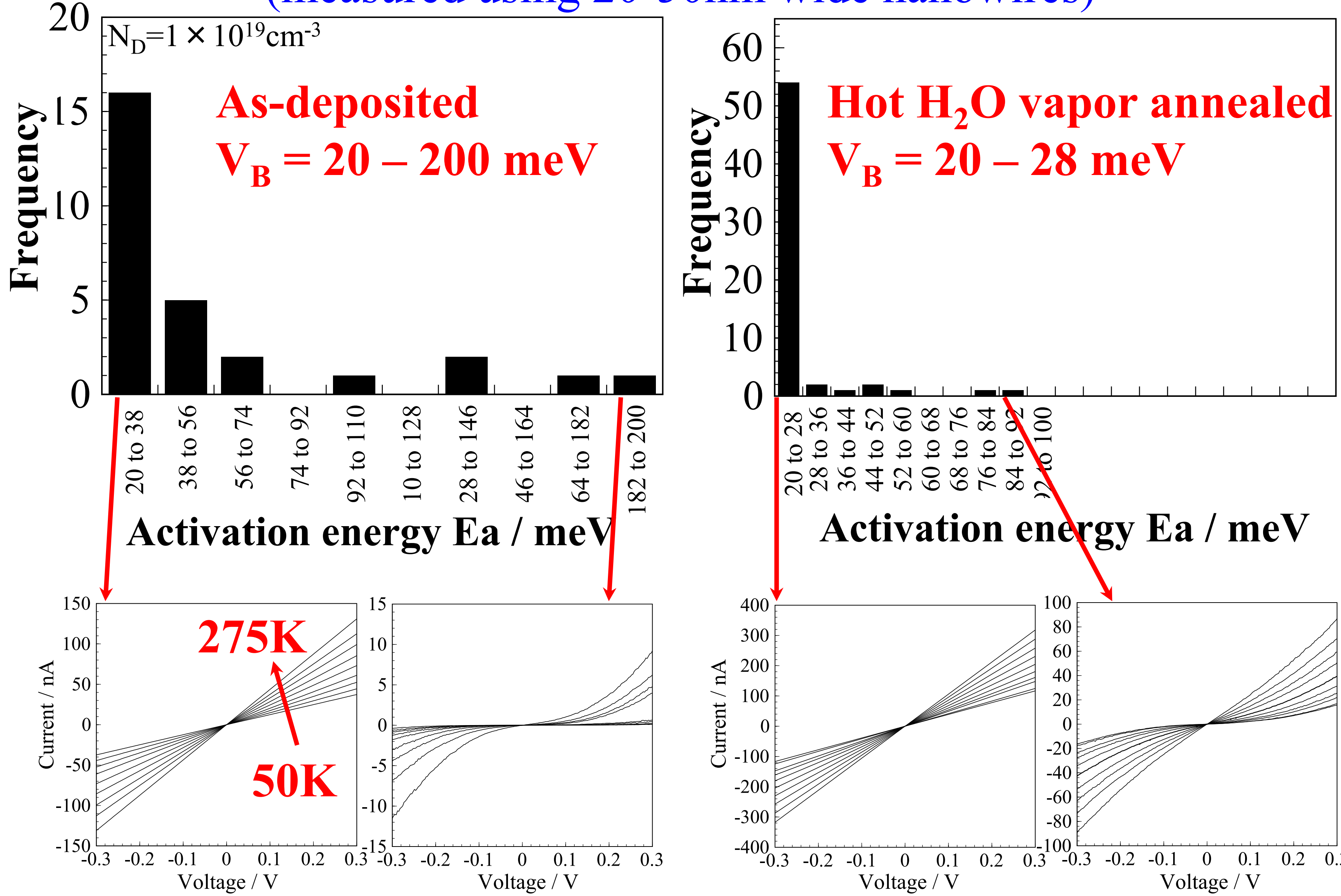


Black: experimental data
Red: fitting results

E_a=10meV-80meV

Distribution in poly-Si GB potential height

(measured using 20-50nm wide nanowires)

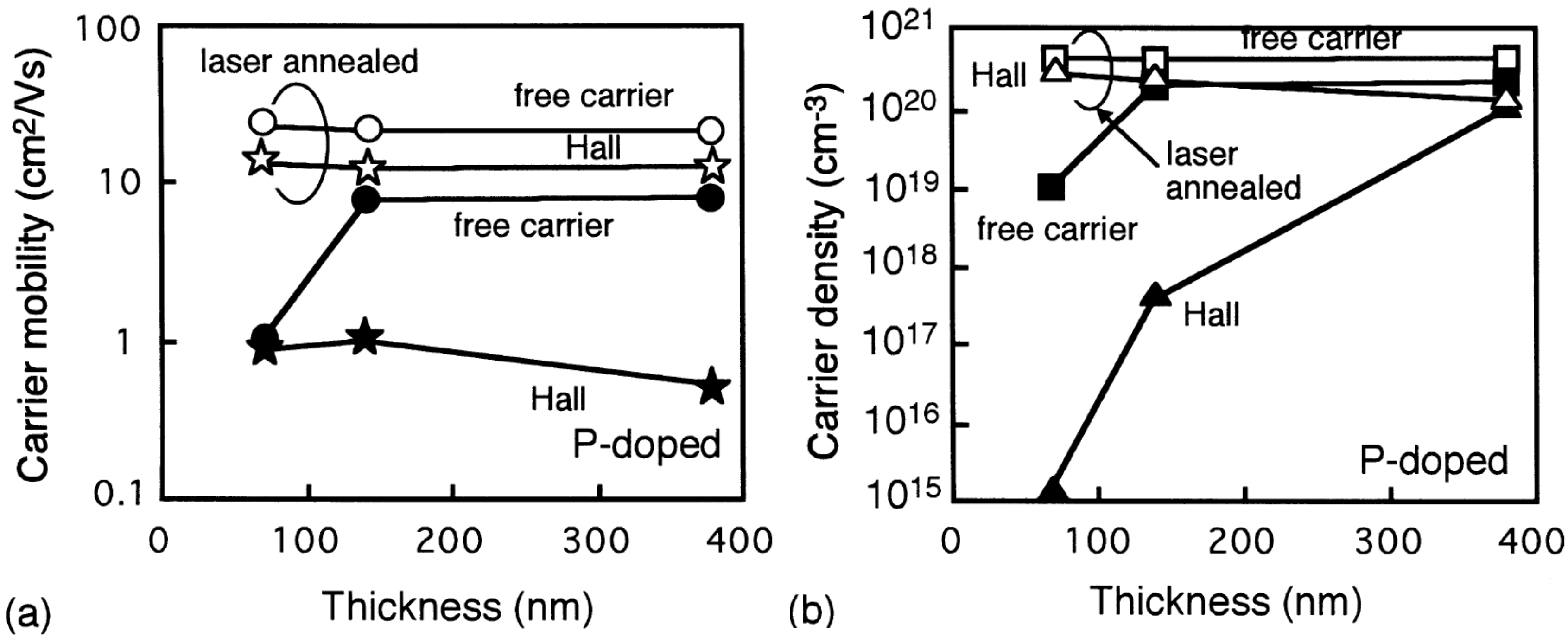


T. Kamiya et al, JVSTB ***21****, 1000(2003)*

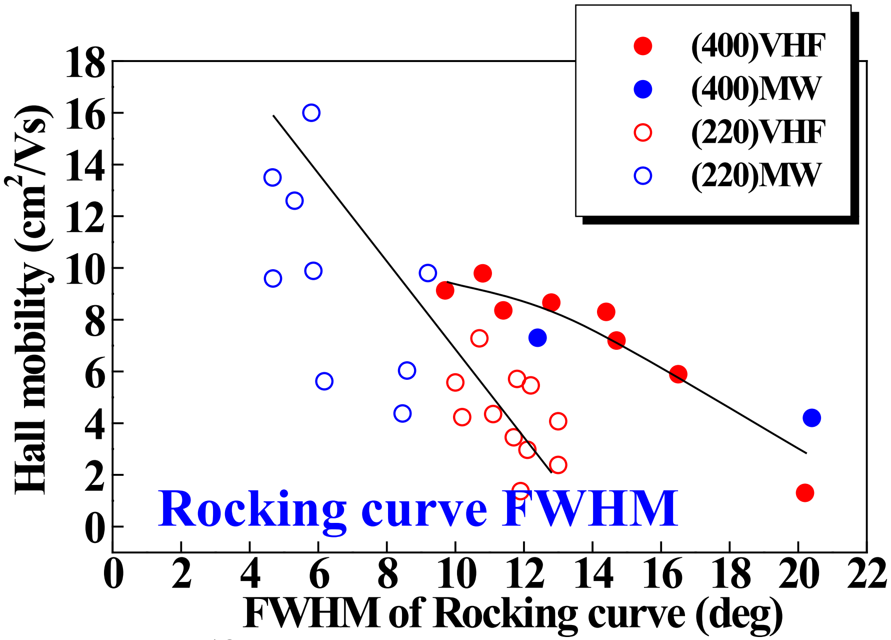
DC mobility (Hall) vs in-grain mobility (FCA)

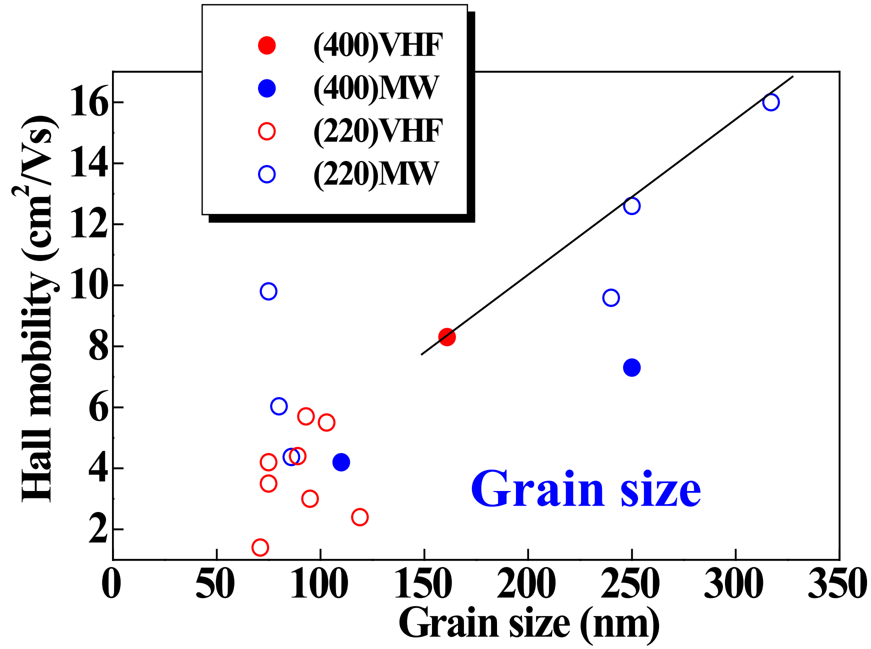
T. Sameshima, K. Saitoh, N. Aoyama, M. Tanda, M. Kondo, A. Matsuda, S. Higashi, Analysis of free-carrier optical absorption used for characterization of microcrystalline silicon films, Sol. Energy Mater. Sol. Cells 66 (2001) 389

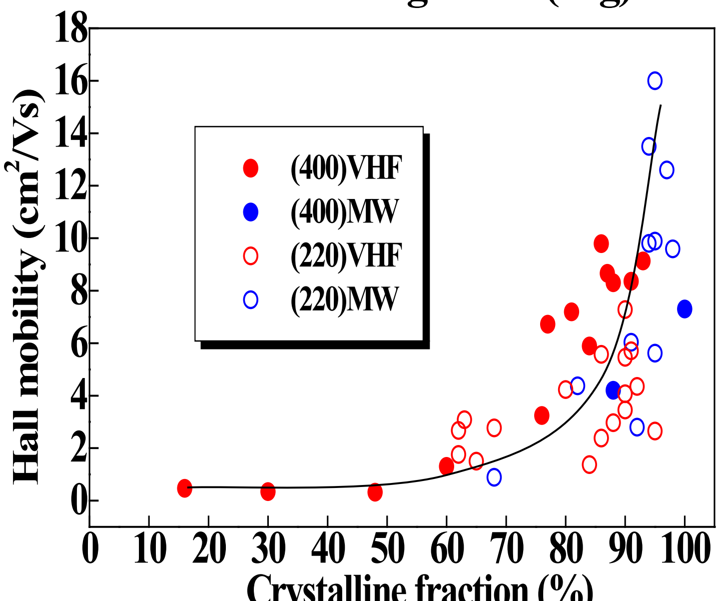
P- / B-doped mc-Si:H: 100 W RF PECVD, 180^{o}C, SIH4/PH3,B2H6/H2
ELA: 28 ns XeCl excimer laser, 160 to 360 mJ/cm^2, 5 pulses



Hall mobility vs microstructures of PECVD mc-Si







Crystalline fraction

Kamiya et al., MRS Proc. **609**, A27.1 (2000)

Electronic conduction in amorphous

アモルファス半導体における電子伝導

Questions for amorphous semiconductors in early years

Bloch's theorem

・ No-scattering electron transport is achieved only for periodic crystals

Electronic structure theory in metal

・Bandgap is formed at BZ boundary by interference of propagation and reflection waves => Bandgap needs priodicity?

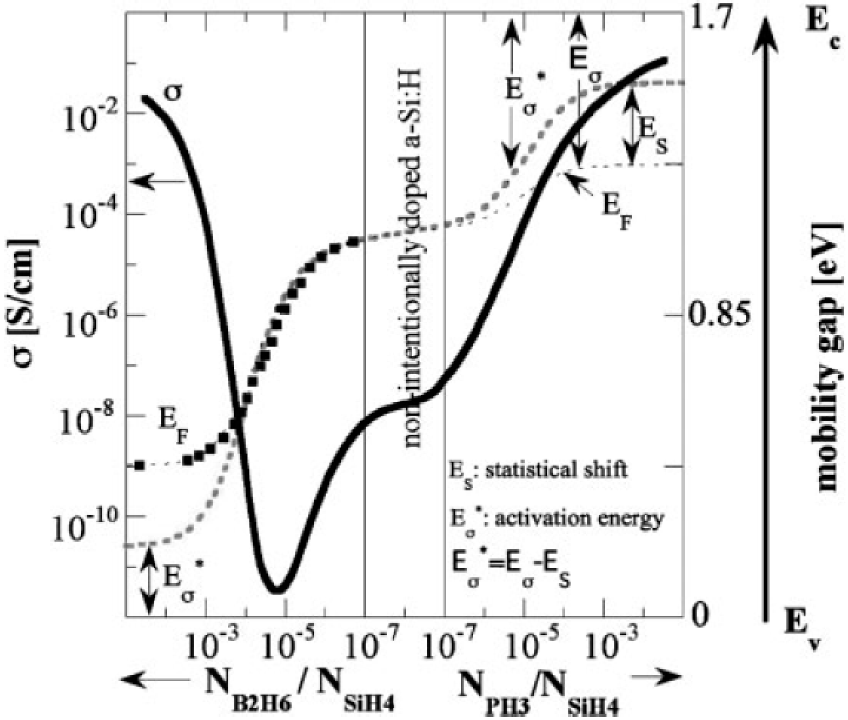
・Why amorphous mater have a finite bandgap?

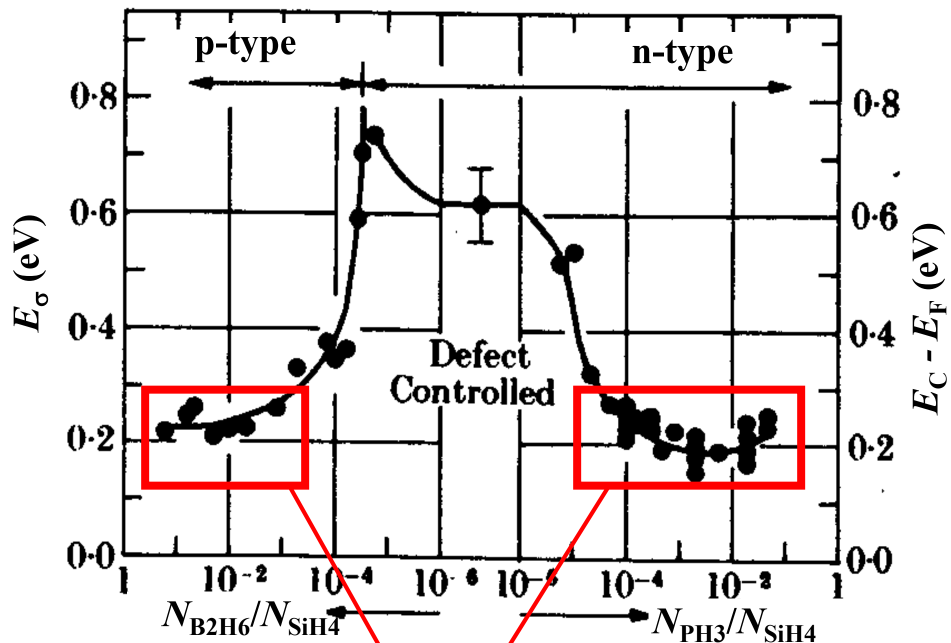
・Why electron conduction is possible in amorphous maters?

・Does effective mass have physical meaning in amorphous maters?

・High mobility amorphous maters are possible?

Conductivity and activation energy of a-Si:H





Activation energy levels off at ~0.2eV:

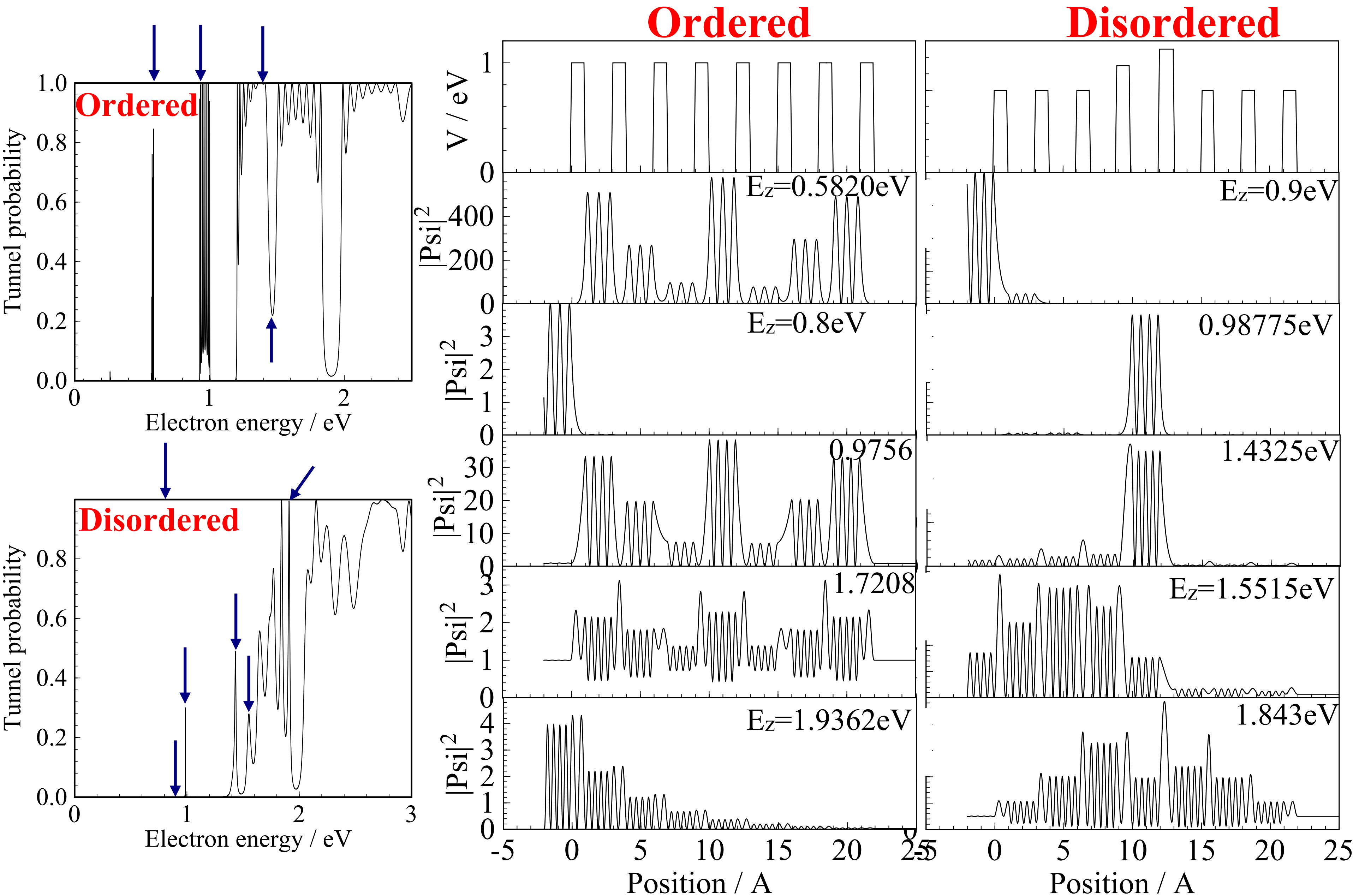
Degenerate conduction never attained

High-density tail-states

Negative-U donor states

W.E. Spear and P.G. LeComber,
Solid State Commun. **17** (1975) 1193

Transmission through disordered MQW



Potential fluctuation and localization

田中一宣他著、アモルファスシリコン、オーム社

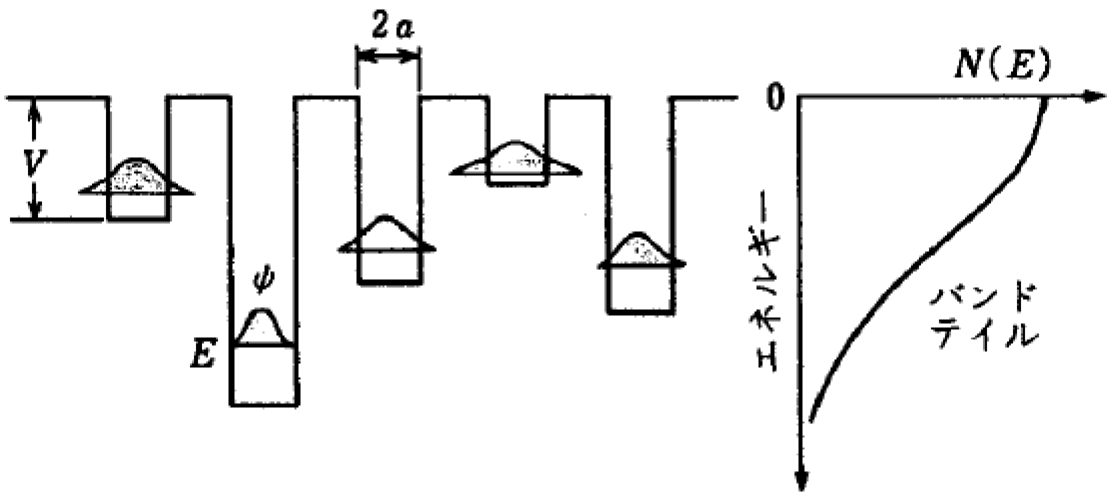
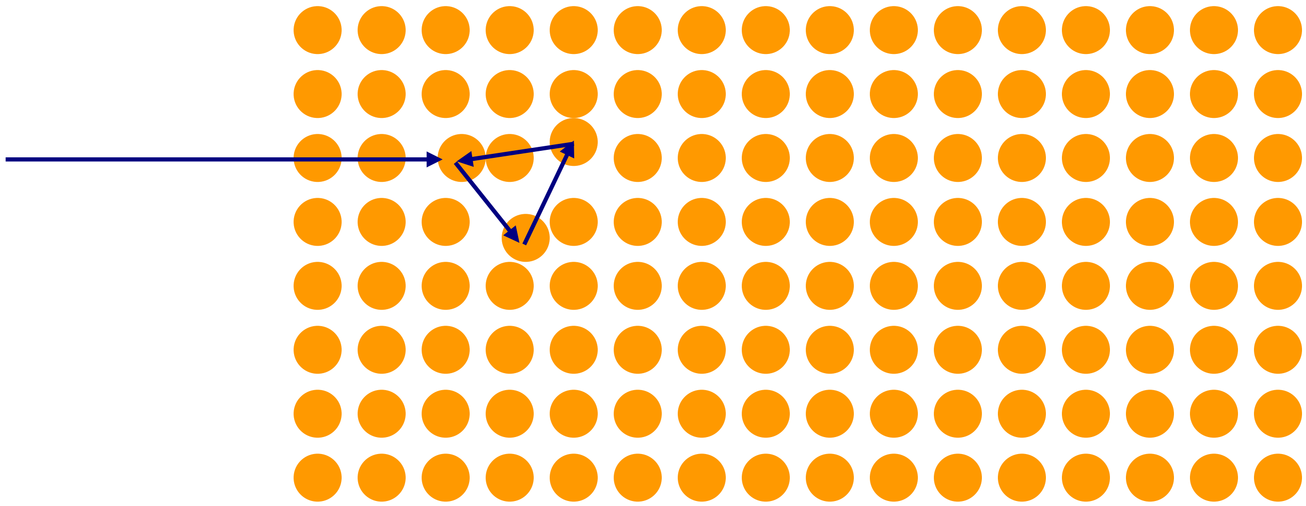
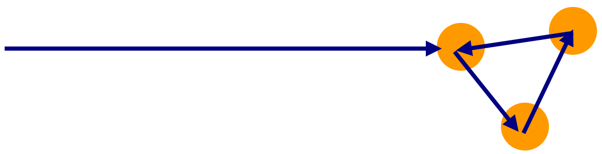


図 4・4　バンド端でのポテンシャルゆらぎの単純化モデルとバンドテイル状態

Transmission through disordered crystal



- **Back ground periodic atoms contribute only to *e*⁻ transmission: we can consider only the difference from the perfect crystal**



- **Due to scattering and interference from the disordered structure, standing wave is formed in a localized region: Anderson localization**

Two hopping conductions

・Nearest-neighbor hopping

Carriers are trapped at localized states, thermally excited and contribute to conduction

$$\sigma = \frac{\sigma_0}{T}\exp\left(-\frac{\Delta E}{k_B T}\right)$$

Carriers are excited by phonons: accompany the lattice deformation

Same as small polaron

⇔ Large polaron:

Carriers move with small lattice deformation,
but not localized and mean free path is larger than lattice period

*** Most of electron conduction in solids form large polaron**
except for non-polar materials like C, Si etc

・Variable-range hopping (VRH)

Carriers are trapped localized states, transferred to other localized states by tunneling
Hopping occurs between distributed energy localized states局在状態のエネルギーに分布があることを考慮するため、ホッピングと呼ばれる

Small polaron

$$S = \pm \frac{k}{e} \ln\left(2 \frac{N-n}{n} \right)$$

N: Total site number able to be occupied by e^-
n: Site number acctually occupied by e^-
Small temperature dependence

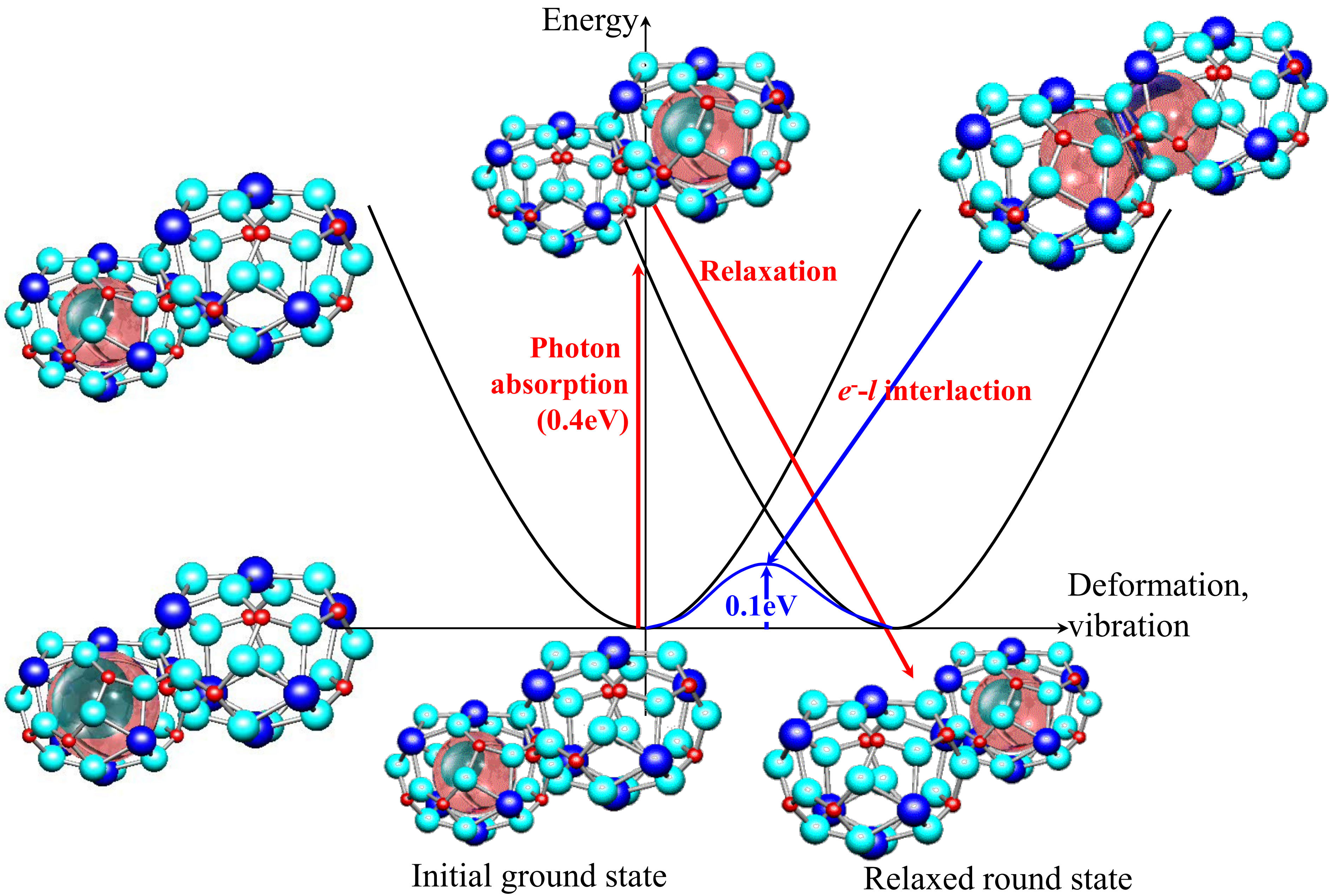
$$\sigma = \frac{\sigma_0}{T} \exp\left(-\frac{E_H}{k_B T} \right)$$

$$\sigma_0 = \frac{gNc(1-c)e^2 a^2 \nu}{k_B}$$

c: n/N
a: Hopping length
ν: Optical phonon frequency contributing to hopping

J. Han, M. Shen and W. Cao, Appl. Phys. Lett., 82 (2003) 67
B.J. Ingram, T.O. Mason, R. Asahi, K. T. Park, A.J. Freeman, Phys. Rev. B 64 (2001) 155114
H. L. Tuller and A. S. Nowick, J. Phys. Chem. Solids **38**, 859 (1977)
J. Nell, B. J. Wood, S. E. Dorris, and T. O. Mason, J. Solid State Chem. **82**, 247 (1989)
H. Böttger and V. V. Bryksin, Hopping Conduction in Solids (VCH Verlagsgesellschaft, Weinheim, Germany, 1985).
A. R. Long, in Hopping Transport in Solids, edited by M. Pollak and B. I. Shklovskii (North-Holland, Amsterdam, 1991).

Polaron conduction in C12A7:e^-



Mott's variable-range hopping (VRH)

- **High defect density so that e^- can tunnel to other defect states**
  => Small temperature dependence due to tunneling
- **Energy distribution in the defects**
  Small temperature dependence
  Hopping distance is varied by temperature => VRH

$$\sigma = \sigma_0 \left(\frac{1}{T} \right)^{1/2} \exp\left[-\left(\frac{T_0}{T} \right)^r \right]$$

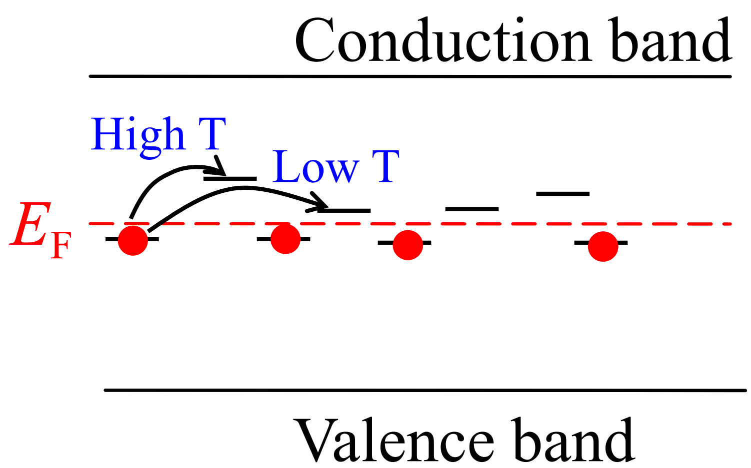
$$\sigma_0 = e^2 \nu_0 \left(\frac{N(E_F)}{32\pi\alpha} \right)^{1/2}$$

$$T_0 = \frac{18\alpha^3}{k_B N(E_F)}$$

$$r = 1 / (d + 1)$$

d: Dimension of the conduction region

r **= 1/4 for 3D VRH**



S.R. Elliott, Physics of amorphous materials, Longman, New York, (1983).
嶋川晃一、林浩司、森垣和夫、広範囲ホッピング伝導ーその大いなる問題点ー、固体物理 29 (1994) 11

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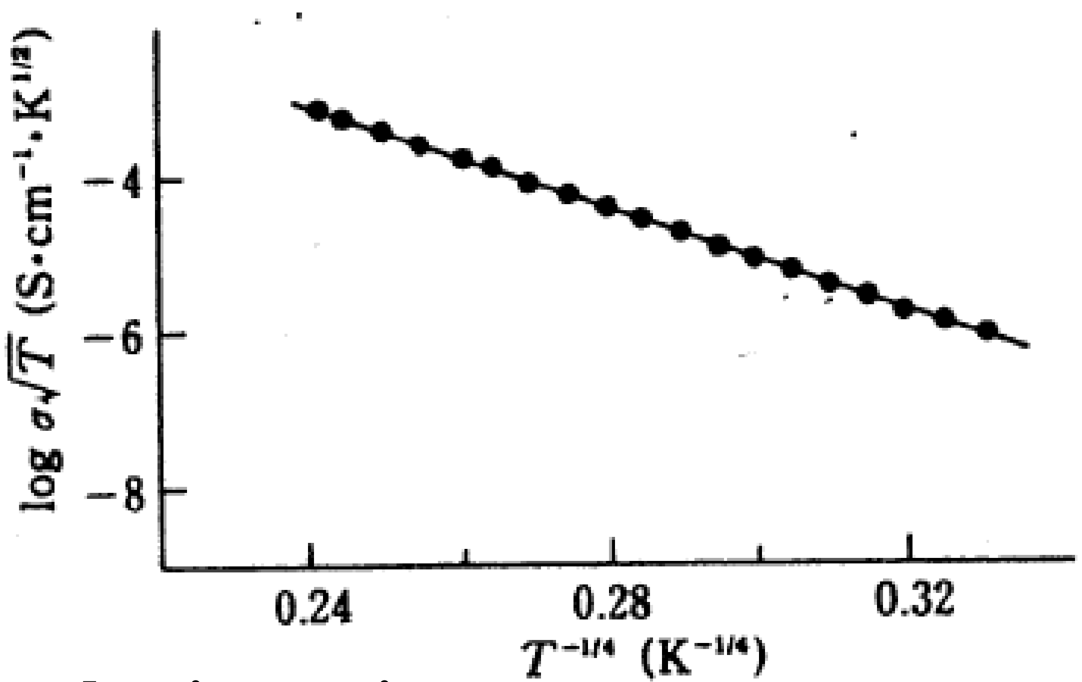
$$T_0 = \frac{18\alpha^3}{k_B N(E_F)}$$

$r = 1 / (d+1)$

d: Dimension of the conduction region

r = ¼ for 3D VRH



S.R. Elliott, Physics of amorphous materials, Longman, New York, (1983).
嶋川晃一、林浩司、森垣和夫、広範囲ホッピング伝導ーその大いなる問題点ー、固体物理 29 (1994) 11

Hall, Seebeck sign anomaly

Amorphous (disordered) semiconductors

- **Inconsistent signs of Hall voltage / Seebeck coefficient with carrier polarity**

  p-type, but negative R_H : pn sign anomaly

  n-type, but positive R_H

  & p-type, but negative R_H : pn sign double anomaly

How to judge carrier polarity with large reliability?

- **For device applications (TFT, FET)**

  C-V, FET

  Problem: Measurable only for good semiconductor/devices

- **Fermi level by photoelectron spectroscopy**

  Problem: Surface band bending

  Resolution (~ 0.1 eV by conventional UPS)

Weak-localization

P.A. Lee and T.V. Ramakrishnan, Rev. Mod. Phys. 57, 287 (1985) through X.D. Liu, E.Y. Jiang, and Z. QW. Li, Low temperature electrical transport properties of B-doped ZnO films, J. Appl. Phys. 102, 073708 (2007)
Kaveh, M., and Mott, N.F. J. Phys. C: Solid State Phys. 14, L177 (1983)

$$\sigma(T) = \sigma_0 + \eta T^{p/2} + \lambda T^{1/2}$$

a phonon scattering model (p = 1)

P.A. Lee and T.V.V Ramakrishnan, Rev. Mod. Phys. 57 (1985) 287
W.Noun,B.Berini,Y.Dumont,P.R.Dahoo,N.Kelle,JAP 102 (2007) 063709

3D limit
$T^{p/2}$: Weak localization (WL), p=2 electron-electron, p=3 electron-phonon interaction
$T^{1/2}$: renomralization of effective electron-electron interaction (REEI)
bT^2: low-T e-e Boltzmann term

$$\rho(T) = \frac{1}{\sigma_0 + \eta T^{p/2} + \lambda T^{1/2}} + bT^2$$

2D limit
ln T for WL and REEI

$$\rho(T) = \frac{1}{\sigma_0 + a \ln T} + bT^2$$

Condition required $\Lambda \sim \lambda_F$

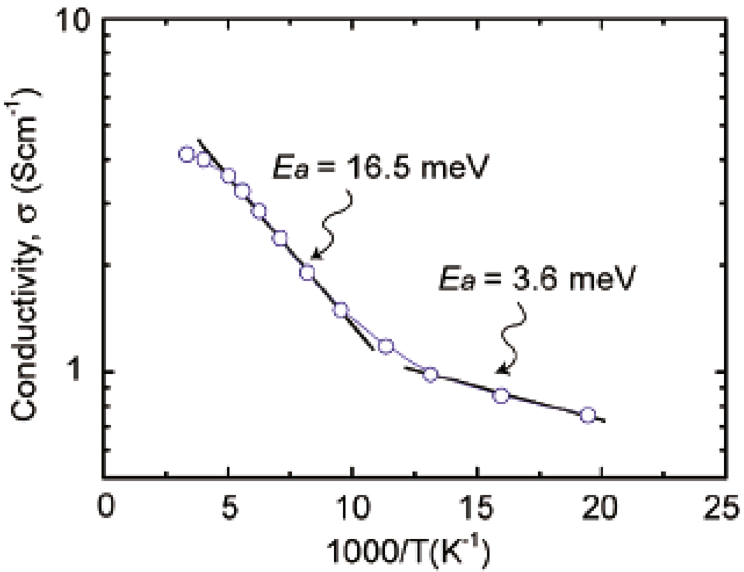
Fermi wavelength $\lambda_F = 2\pi / (3\pi^2 n)^{1/3}$

Electron mean free path $\Lambda = h / (\rho n e^2 \lambda_F)$

Percolation conduction

Percolation伝導

Mott's variable-range hopping (VRH) ?



ZnO film/SCAM substrait
Non-straight line in Arrhenius plot
=> better fit to VRH

T_0 & σ_0 => α^{-1} = 0.6 nm, $N(E_F)$ = 3.1 × 10^{22} cm^{-3}/eV
$N(E_F)$ (defect density at E_F in the bandgap) is extraordinarily large => Other model

- **VRH often provides very high σ_0 (several order larger than common sense) (Prefactor problem)**
- **It is accepted not to discuss σ_0**
- **VRH is not compatible with conventional Hall theory**

嶋川晃一、林浩司、森垣和夫、広範囲ホッピング伝導ーその大いなる問題点ー、固体物理 29 (1994) 11
杉原硬、広範囲ホッピング伝導、固体物理 12 (1977) 15

第1表 Mottの広範囲ホッピング(1/4乗則).

	T_0 (K)	σ_0 (S·cm^{-1})	α^{-1} (cm)	$N(E_F)$ (cm^{-3}·eV^{-1})	
				T_0より計算	σ_0より計算
c-Si(イオン打ち込み)	48	1.9×10^2	4×10^{-6}	7×10^{19}	2×10^{21}
c-Ge(N_d=1.5×10^{17} cm^{-3})	1.9×10^4	1.9×10^4	7×10^{-7}	3×10^{19}	2×10^{24}
a-Si	3.5×10^7	9.6×10^3	1×10^{-7}	6×10^{18}	3×10^{26}
a-$Si_{100-x}Au_x$ (x=2.4)	2.8×10^7	3×10^9	1×10^{-7}	8×10^{18}	3×10^{37}
V_2O_5–P_2O_5 ガラス	2.8×10^9	2×10^{17}	4×10^{-8}	7×10^{17}	4×10^{53}
PCBCO 薄膜	2.9×10^5	1.8×10^4	1×10^{-7}	7×10^{20}	1×10^{25}

参考文献: シリコン単結晶(c-Si)[文献26], ゲルマニウム単結晶(c-Ge)[文献4], アモルファスシリコン(a-Si)[文献23], アモルファスシリコン-金(a-$Si_{97.6}Au_{2.4}$)[文献24], V_2O_5–P_2O_5ガラス[文献21], 高温超伝導体(PCBCO)薄膜[文献27]. 上記$N(E_F)$はすべてMottの式(§2)で計算された.

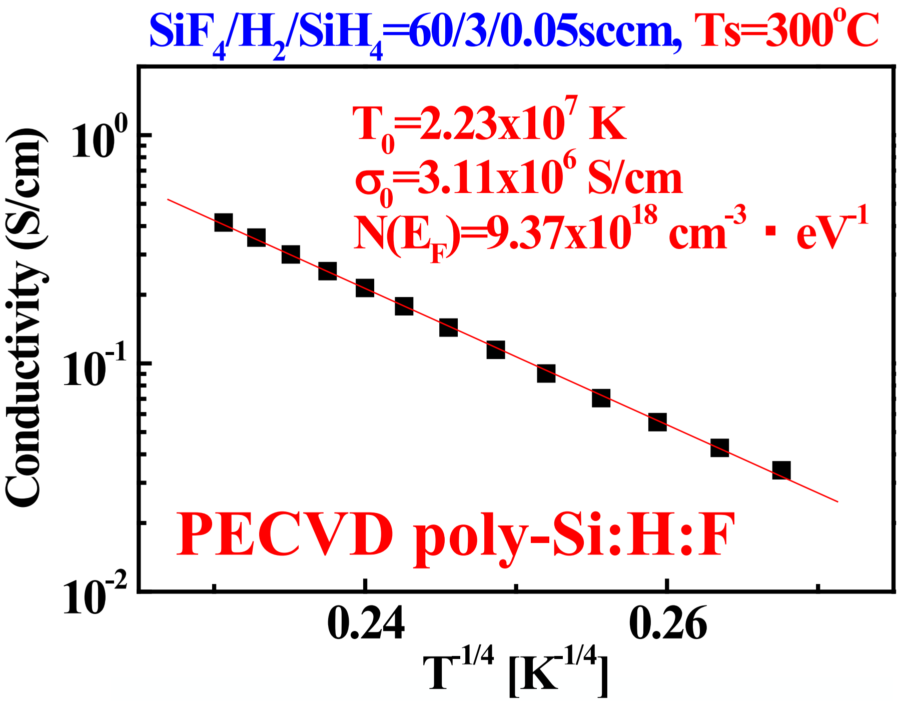
Sir Nevill Mott also pointed …

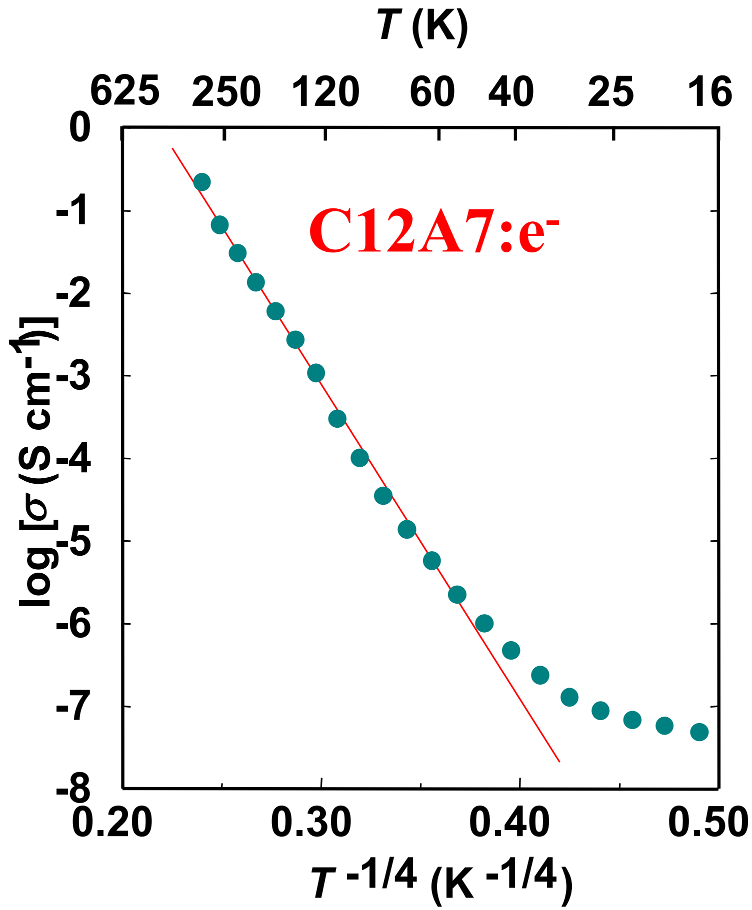
e.g. in *Conduction in Non-Crystalline Materials (1993)*

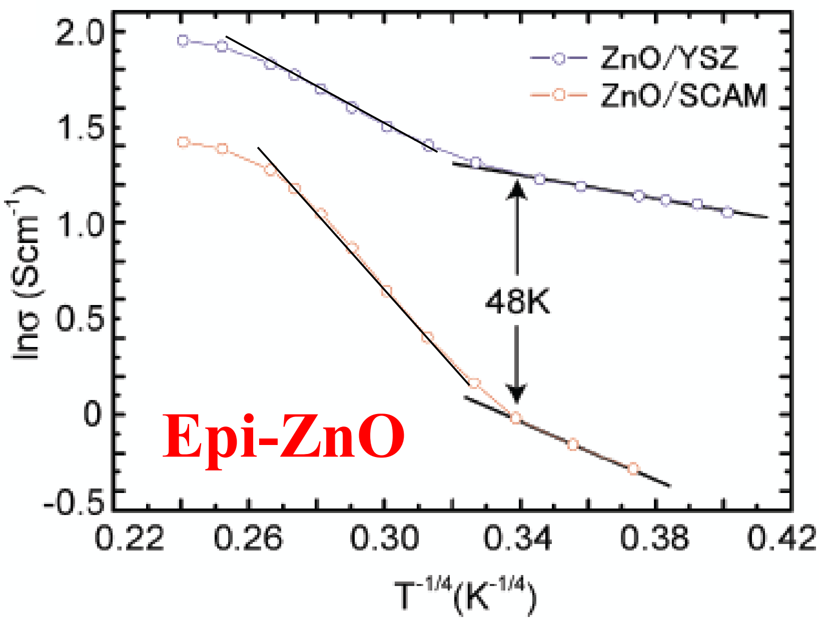
Conduction in granular metals | 35

In this section we have used elementary arguments to obtain the $T^{1/4}$ and $T^{1/2}$ laws. For a more accurate percolation method, which gives almost the same results, see Ambegaokar *et al.* (1971) and Pollak (1972). More recently Sivan *et al.* (1988) and others have argued that the percolative-like nature of the charge transport in these systems can give rise to a nonlinear averaging process that may cause a negative magnetoresistance. Effects on thin films are anticipated and have been investigated experimentally (Ovadyahu 1986; Erydman *et al.* 1992).

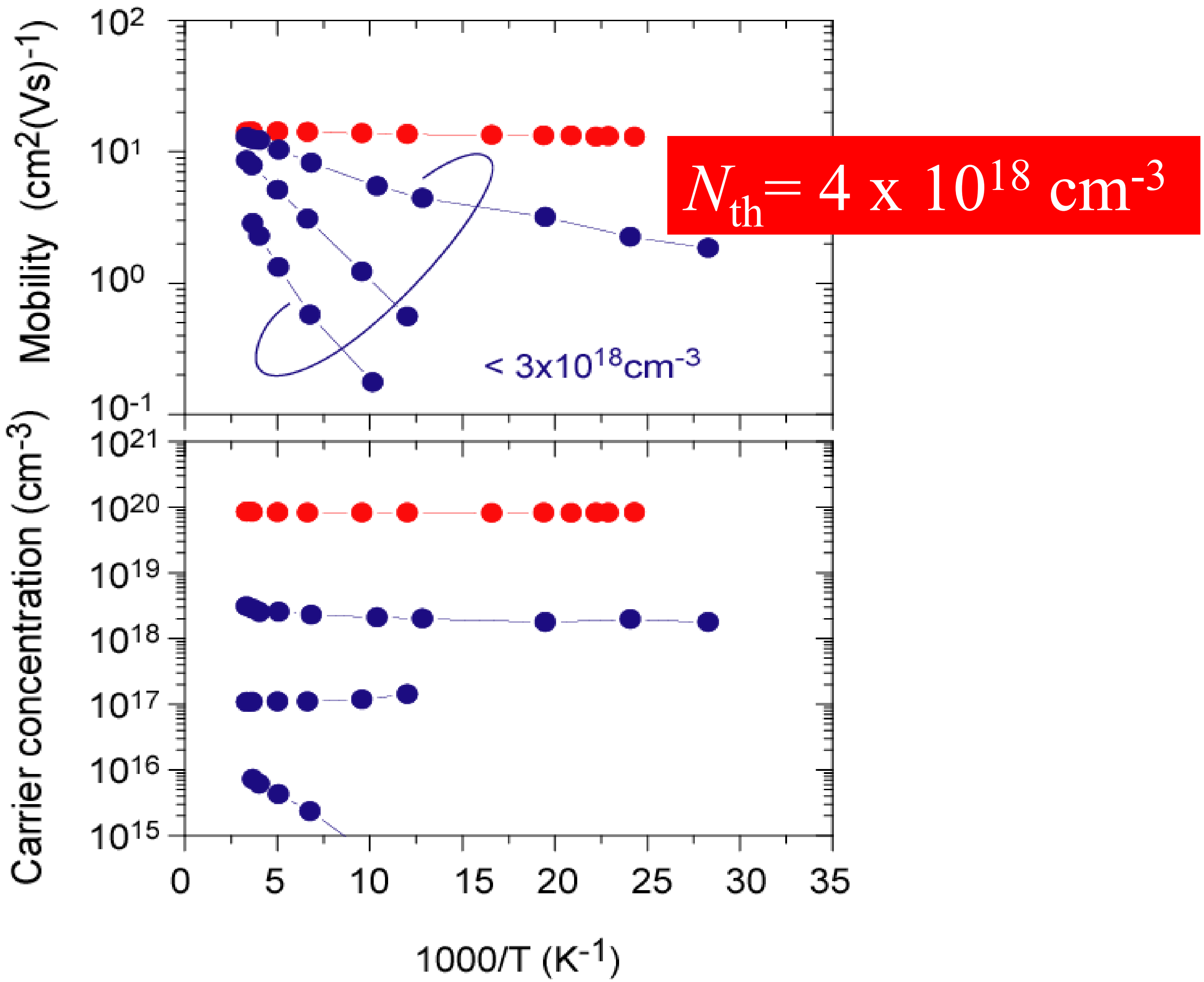
VRH everywhere in poor semiconductors ???







Carrier transport in a-IGZO



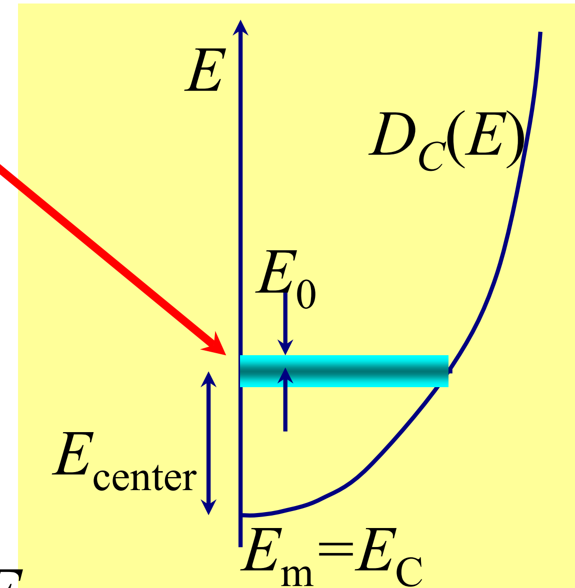
Degenerate conduction both in N_e and μ_e at $N_e > 4\times10^{18}$ cm^{-3}

Perolation model

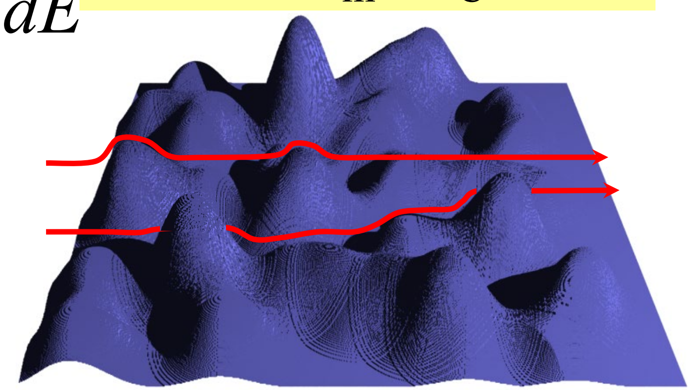
$$\sigma_x = -\frac{2e^2}{3m_e}\int (E - E_m)\tau(E)D(E)\frac{\partial f_0}{\partial E}dE = en_e\frac{e}{m_e^*}\langle \tau^1 \rangle$$

$$g(E) = \exp\left\{-(E - E_{center})^2 / E_0{}^2\right\}$$

$$p(E) = \left(\pi E_0{}^2\right)^{-1/2}\int_E^{\infty} g(E')dE'$$



$$\sigma_x = -\frac{2e^2}{3m_e}\int (E - E_m)\tau(E)p(E)D_C(E)\frac{\partial f_0}{\partial E}dE$$



$$n_e = \int_{E_C}^{\infty} D_C(E)f_e(E)dE$$

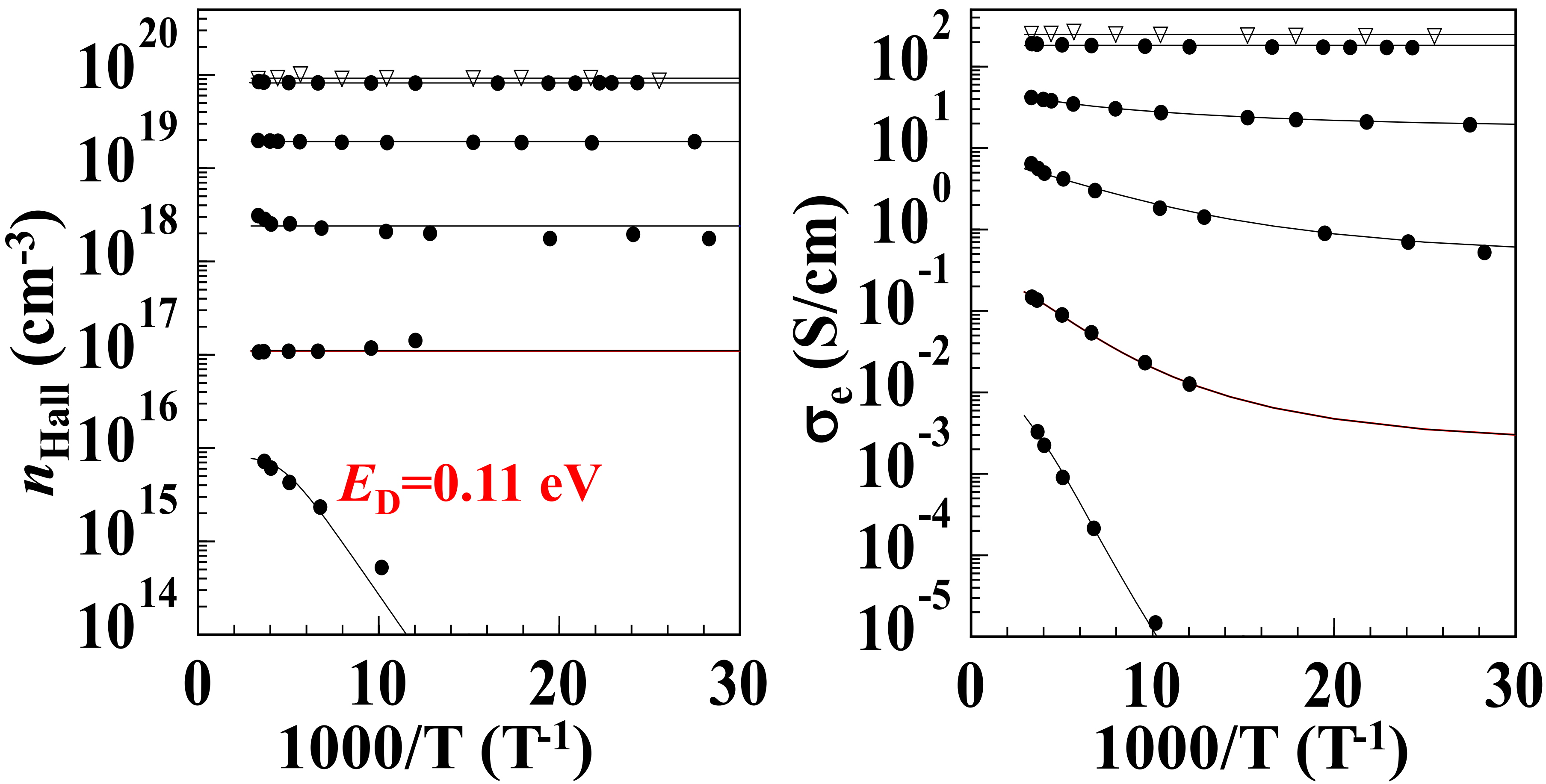
$$F_{Hall} = \langle \tau^2 \rangle / \langle \tau^1 \rangle^2$$

$$n_{Hall} = n_e / F_{Hall} \qquad \mu_{Hall} = \mu_e F_{Hall}$$

Hall results vs percolation model: a-IGZO

r=0.5

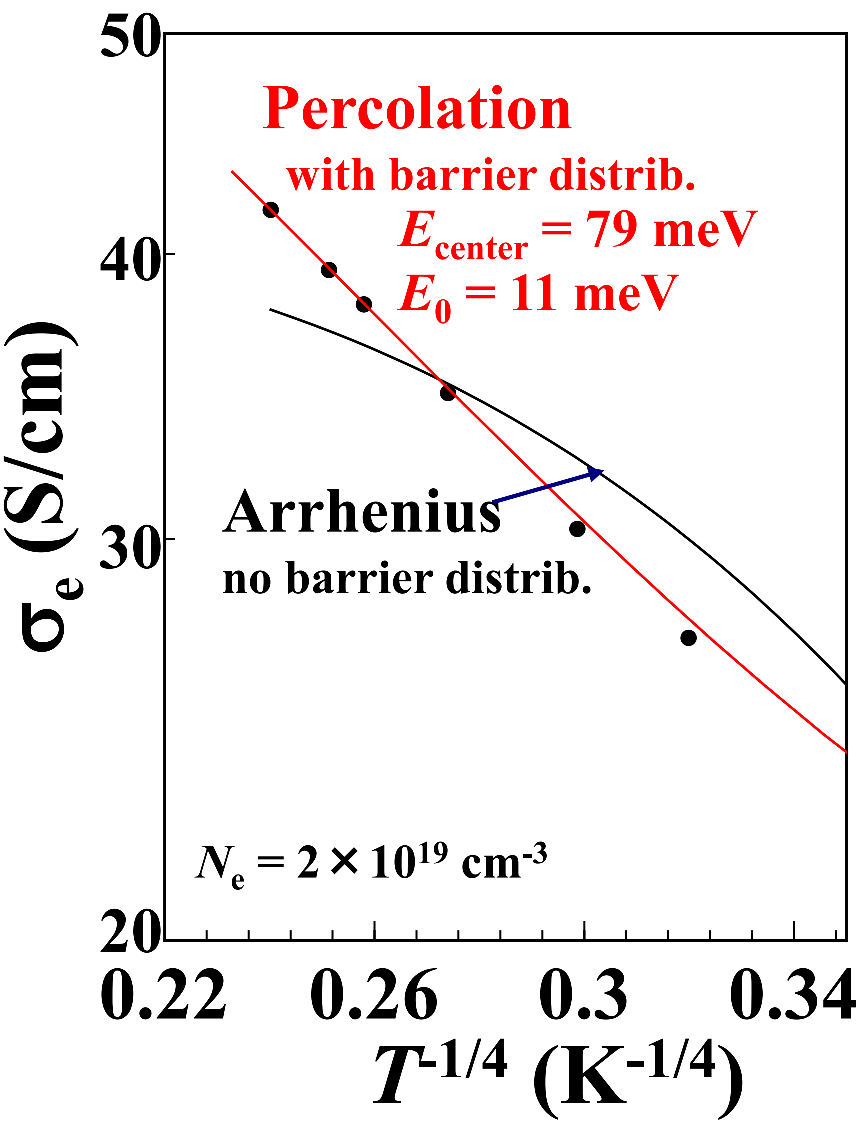
Kamiya et al., J. Dipl. Technol.**5**, 462 (2009)
Kamiya et al., APL 96, 122103 (2010)

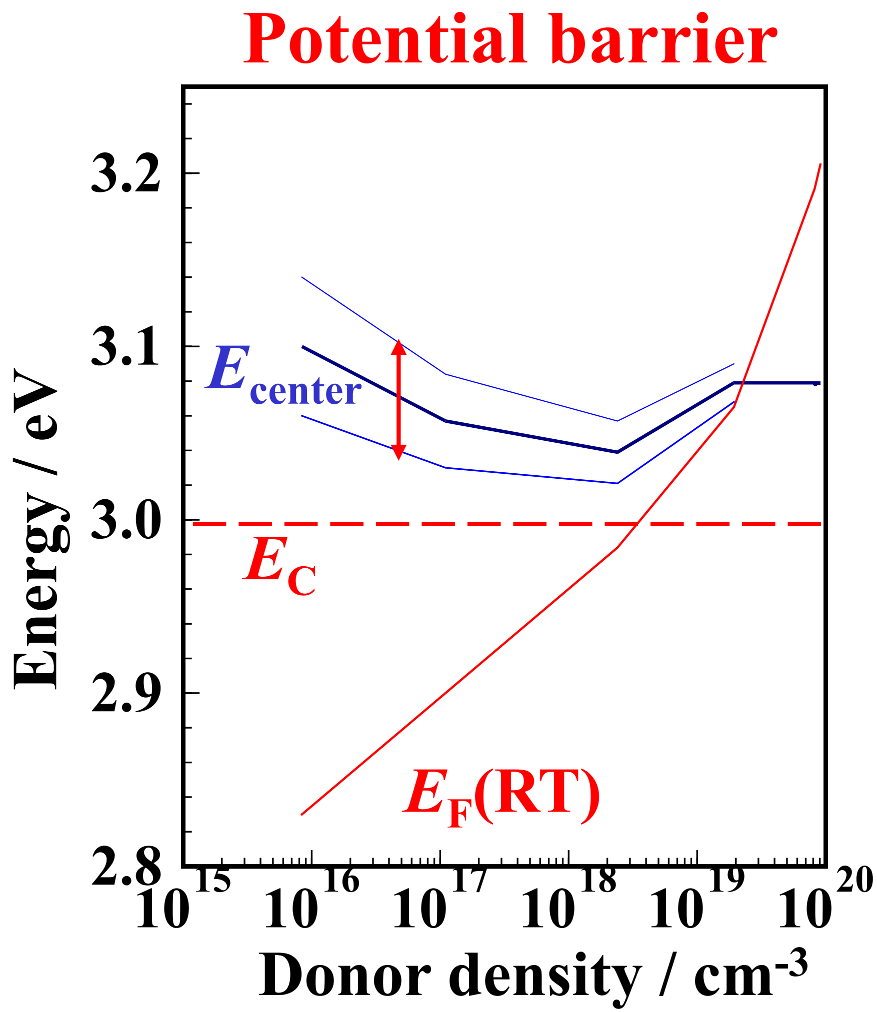


$T^{-1/4}$ behavior and potential barriers

Kamiya et al., APL 2010

a-IGZO

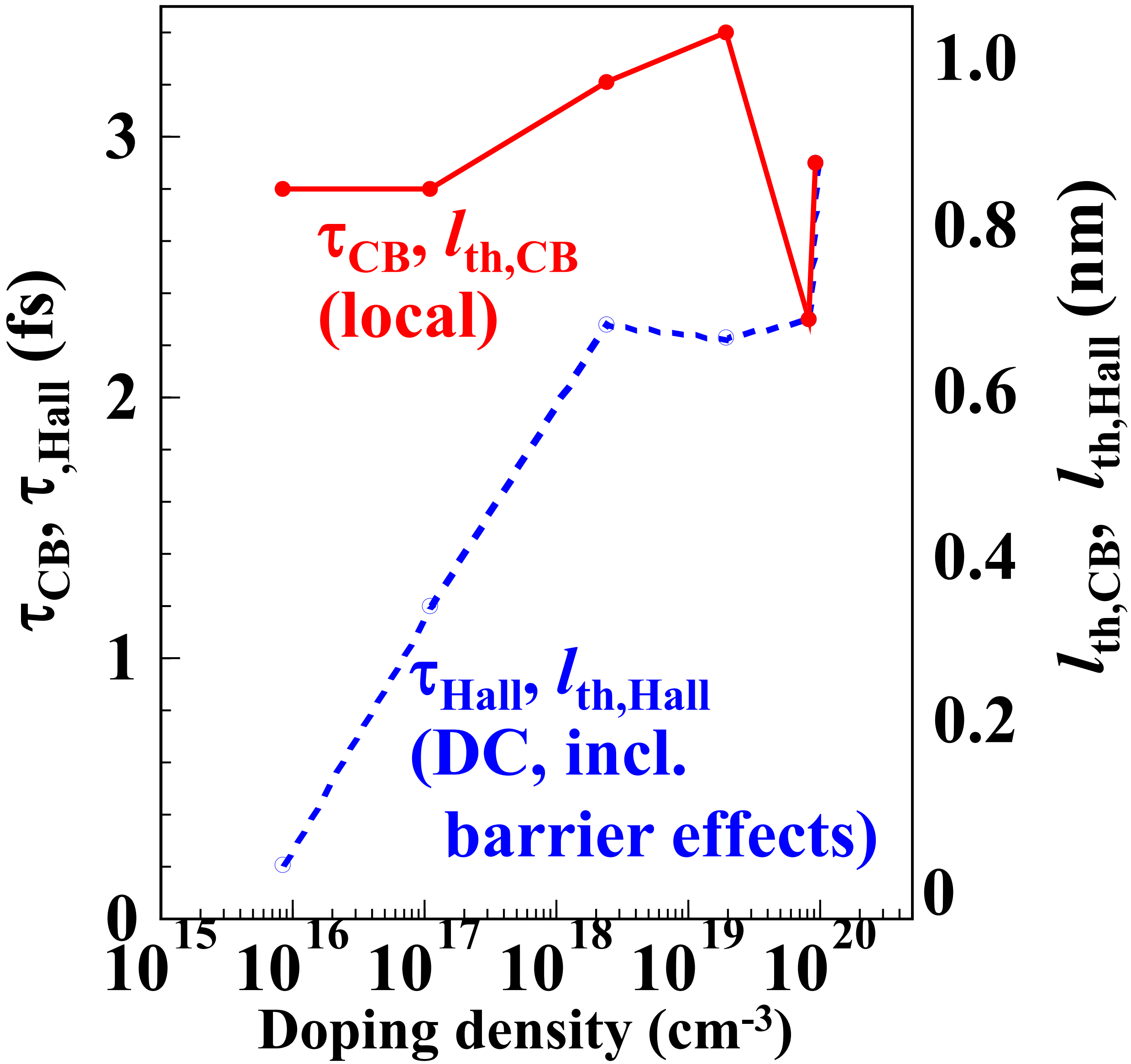


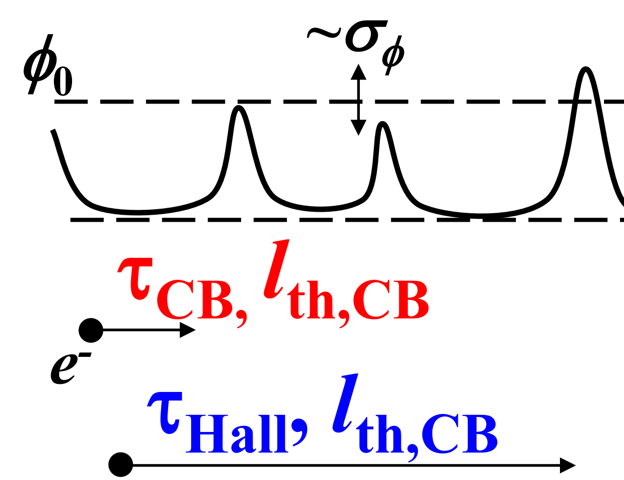


Local and global mean free path

Kamiya et al., APL 2010

300 K, $m = 0.35\ m_e$ **r=0.5**





Ambiguity in mobility

$\sigma = en\mu$

Only σ is defined without ambiguity.

Drift mobility: $\mu_d = \mu_{drift}/E$ **Definition in physics**

Conductivity mobility: $\sigma = en\mu$

μ value depends on the choice of n.

n: Hall effect => Hall mobility

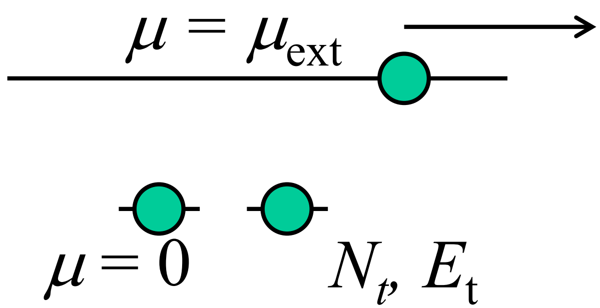
Optical absorption => Optical mobility

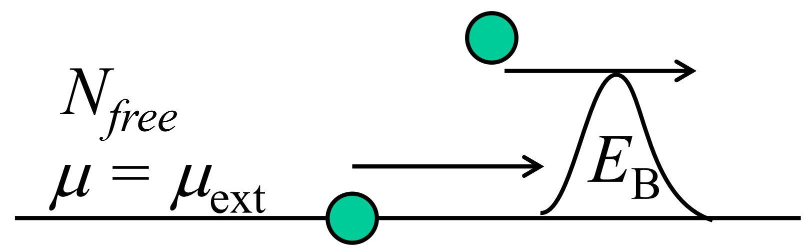
Field effect => FE motility

Case of inhomogeneous materials?

$N_B = N_{free}\exp(-E_B/kT)$

$N_{free} = N_t\exp(-E_t/kT)$





$\mu = \sigma / N_{free}$ or σ / N_B

$\mu = \sigma / N_t$ or σ / N_{free}