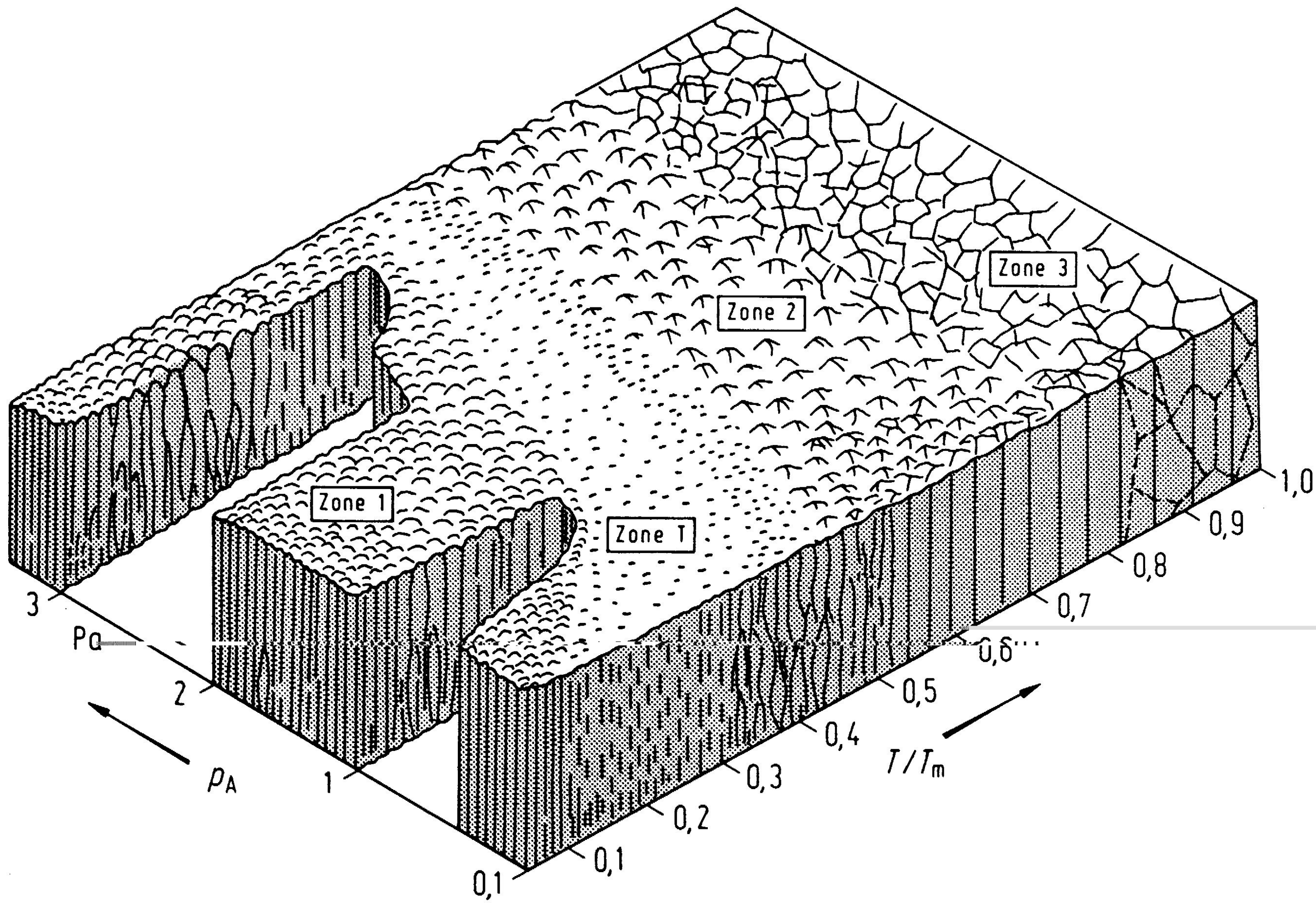
Repetition: Structure Zone Models



Repetition: Film Growth Mechanisms

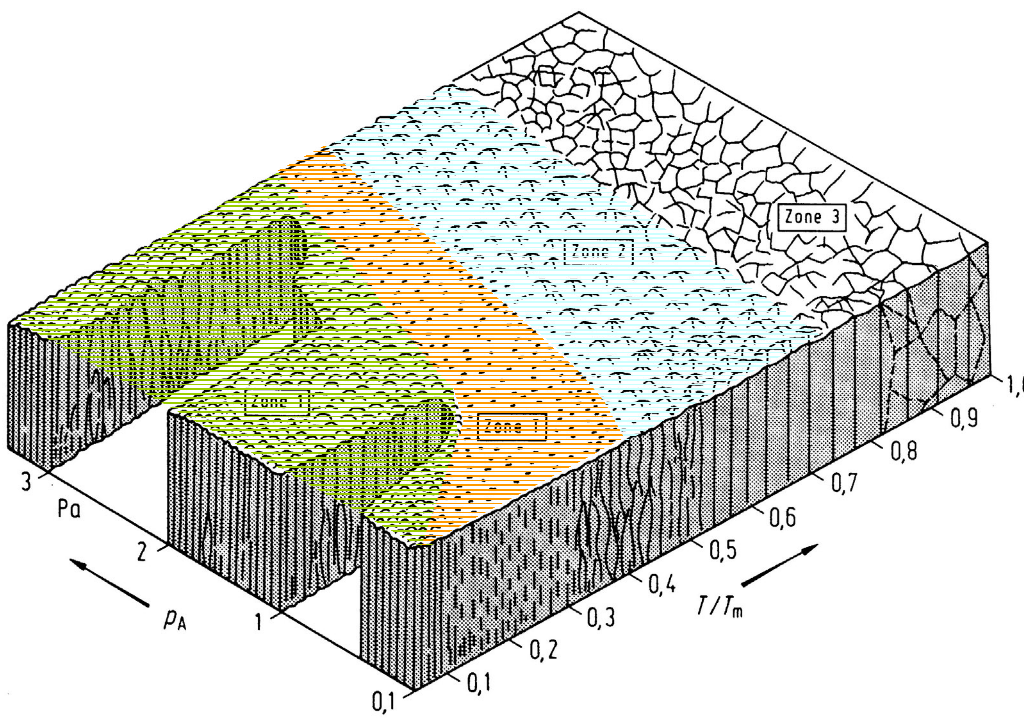
Zone	Mechanism	Char. feature
1: $T/T_M<0,2$	Shadowing	Fibers, pores
T: $T/T_M<0,4$	Particle energy	Nano grains
2: $T/T_M<0,8$	Surface diffusion	Columnar crystlites
3: $T/T_M>0,8$	Volume diffusion	3d - Grains

Repetition: Stress/Film Structure

Intrinsic stress:

σ_I

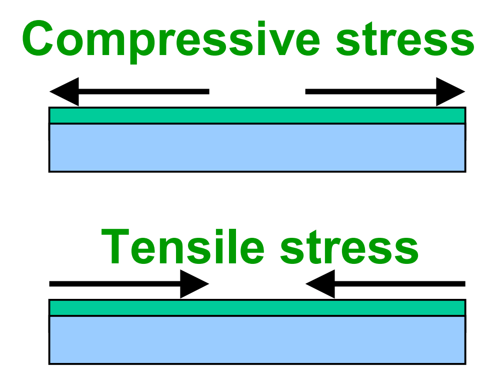
Intrinsic stresses are a direct consequence of the film structure and of the deposition conditions.



Tensile stress

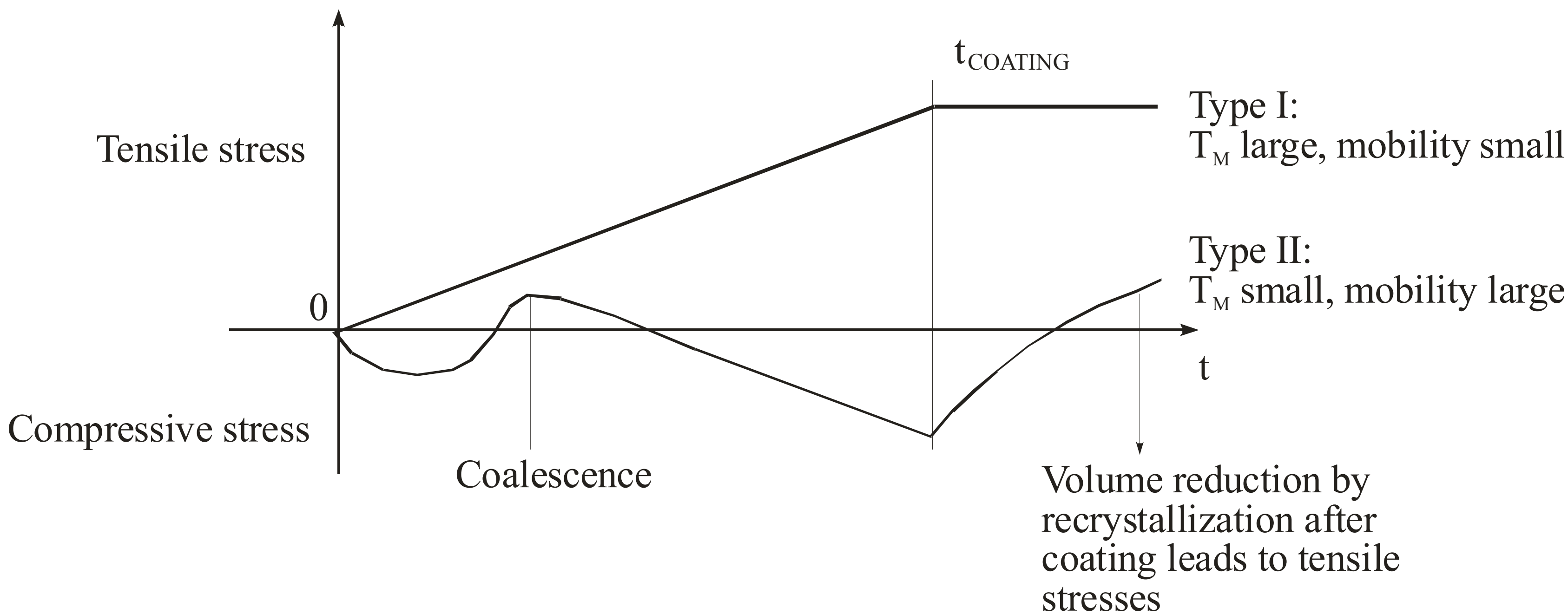
Compressive stress

Variable



Repetition: Stress/Film Growth

In-Situ-measurements by the cantilever method:



Influence of the film thickness on σ_I

Electronic Properties

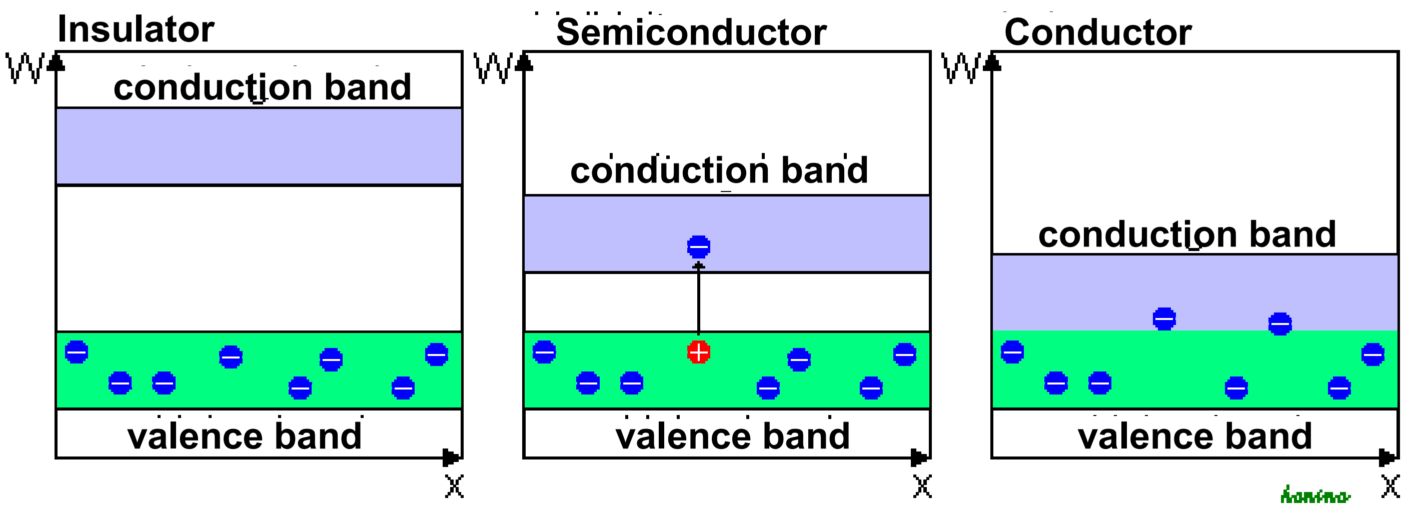
The properties of the electronic system of a meterial exert an influence on:

- **+ Conductivity**
- **+ Optical properties**
- **+ Magnetic properties**
- **+ Adsorption and adhesion**

For thin film systems these properties are furthe modified by the high ration of surface to volume.

Material Classes and Conductivity

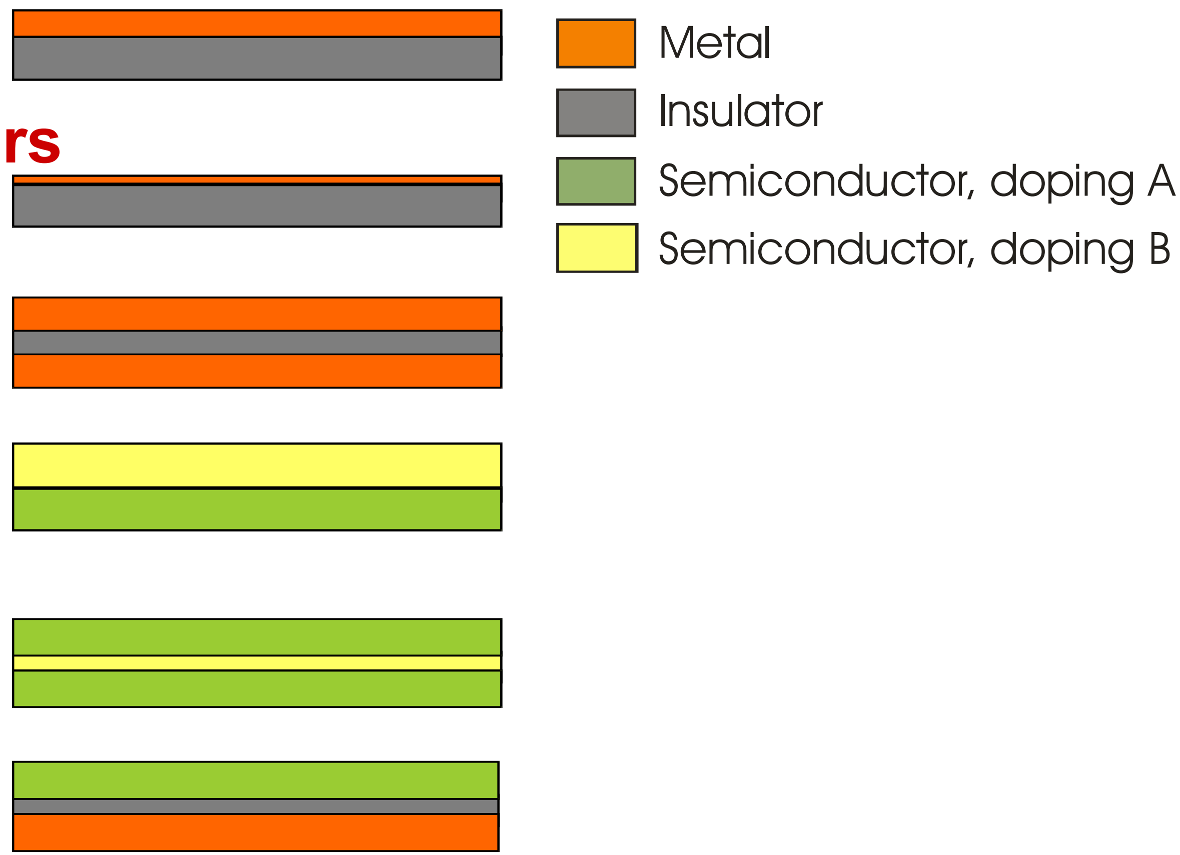
Different material classes may be distinguished by the band model. Basically this model describes the transition from covalent to metallic bonding.



Electronic Components and Thin Films

By thin film technology the following electronic components can be realized:

- **+ Interconnect**
- **+ Thin film resistors**
- **+ Condensers**
- **+ Diodes**
- **+ Transistors**
- **+ MOSFETS**



Electrical Conductivity of Metals

Macriscopic description: Ohm's law

$$I = \frac{U}{R}$$

I = Current
U = Voltage
R = Resistivity

Microscopic description: Drude law

$$\vec{j} = \frac{ne^2\tau}{2m_e}\vec{E} = \sigma \cdot \vec{E}$$

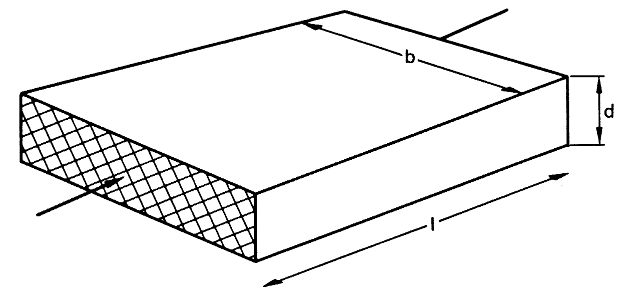
j = Current density
E = E-field
σ = Conductivity
n = Number of charges
e = Elementary charge
m_e = Electron mass
τ = mean collision time

Areal Resistivity

Geometry and electrical resistivity:

$$R = \rho \frac{l}{d \cdot b}$$

ρ= Specific resistivity



An important quantity in thin film technology is the areal resistivity: for l=b (quadratic base area)

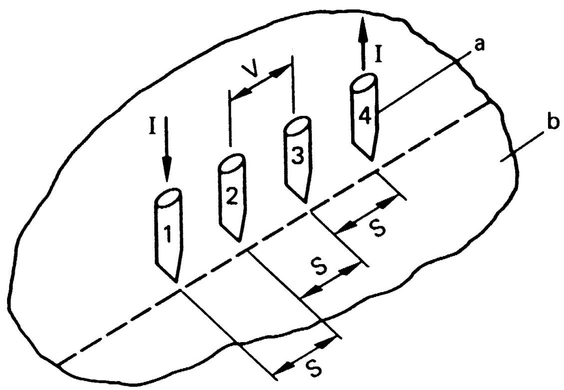
$$R = R_{\square} = \frac{\rho}{d}$$

Is valid independent from the size of the square.

Measurement of the Areal Resistivity

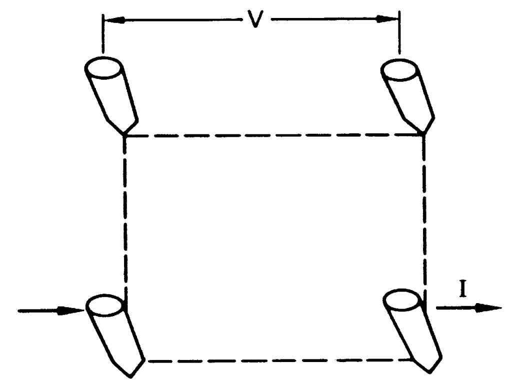
Four point methods:

linear



$$R_{\square} = 4{,}532 \cdot \frac{U}{I}$$

quadratic



$$R_{\square} = 9{,}06 \cdot \frac{U}{I}$$

+ The electrode distance has to be much smaller than the film area.
+ Pre-factors result from electrode geometry.
+ Four pount probes are usually calibrated.

Theory of Conductivity

Drude theory:

$$\vec{j} = \frac{ne^2\tau}{2m_e}\vec{E} = \sigma \cdot \vec{E}$$

j = Current density
E = E-field
σ = Conductivity
n = Number of charges
e = Elementary charge
m_e = Electron mass
τ = Mean collision time

The central point of the Drude theory is the

Mean collision time τ

The Mean Collision Time

The mean collision time can be calculated from "Matthiessens rule":

$$\frac{1}{\tau} = \frac{1}{\tau_G} + \frac{1}{\tau_K} + \frac{1}{\tau_V} + \ldots$$

τ_G **= Scattering at lattice atoms**
τ_K **= Scattering at grain boundaries**
τ_V **= Scattering at impurities**

Important for the magnitude of conductivity is therefore the kind and number of defects, at which electrons can be scattered.

Also interfaces of each kind can be considered as defects. This automatically yields the dependence of the conductivity on film thickness!

Conductivity and Transport Theory

For a mathematically correct and also for a quantum mechanically sound calculation of the conductivity of solid bodiesor thin films Boltzmann's transport theory has to be applied.

Conductivity Without E-field

General approach for the calculation of the conductivity in metals:

Starting point: current density

$$\vec{j}_e = -ne\vec{v} = -e\vec{v}\int_N \frac{dn}{V} = -e\vec{v}\frac{N}{v} = -ne\vec{v}$$

$$dn = 2 \cdot f_0(E) \cdot d\Phi$$

$$f_0(E) = \frac{1}{1 + e^{(E - E_f/k_B T)}}$$

Fermi-distribution

$$d\Phi = \frac{d^3x d^3p}{h^3}$$

Phase space volume, number of states in the phase space volume element $d^3x d^3p$

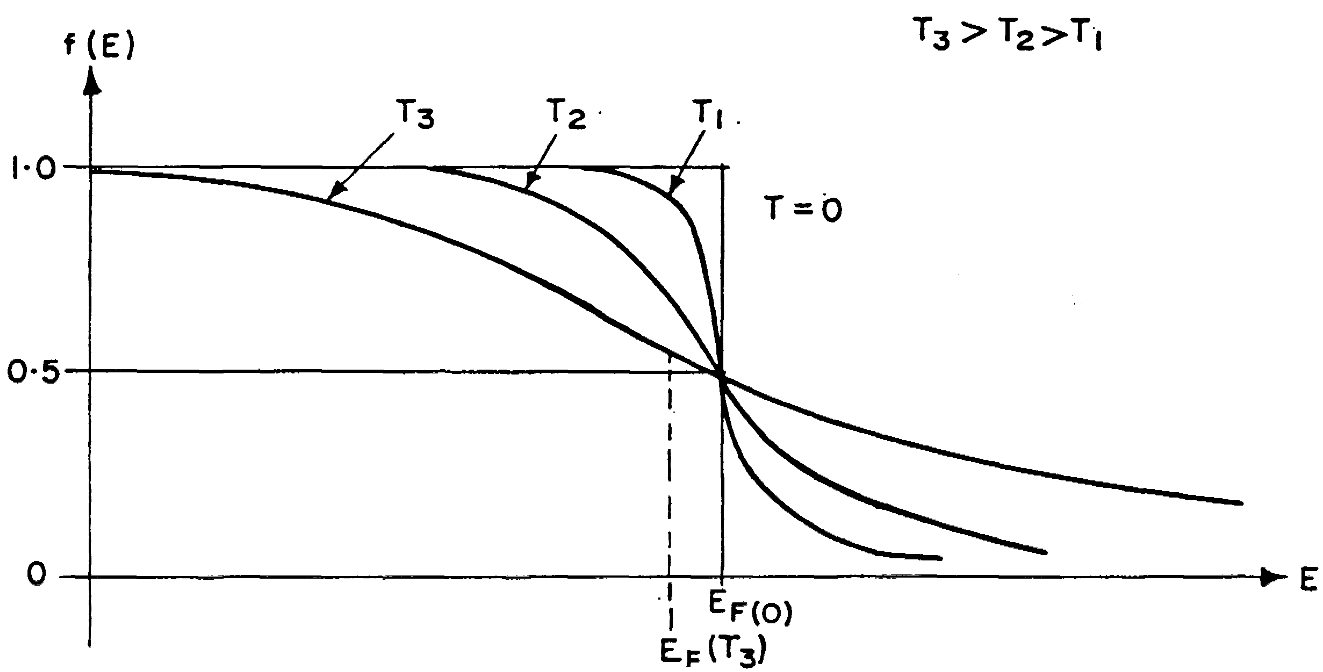
2

Spin-number

Structure of the Fermi Distribution

Ungestörte Fermi-Verteilung:

$$f_0(E) = \frac{1}{1 + e^{(E - E_f / k_B T)}}$$



Calculation of the Current Density I

No E-Field means no disturbance of theFermi distribution:

$$f_0(\vec{v}) = \frac{1}{1+e^{\left[\left(mv^2/2 - mv_f^2/2\right)/k_B T\right]}}$$

$$\vec{j}_e = -e\int_{R,\vec{v}} \vec{v}\frac{dn}{V} = -2e\int_{R,\vec{v}} \vec{v} f_0(\vec{v})\frac{d\Phi}{V} = \left| d\Phi = \left(\frac{m}{h}\right)^3 d^3x d^3v \right| =$$

$$-2e\left(\frac{m}{h}\right)^3 \frac{1}{V} \cdot \int_{\vec{R}} d^3x \int_{\vec{v}} \vec{v} f_0(\vec{v}) d^3v = -2e\left(\frac{m}{h}\right)^3 \int_{\vec{v}} \vec{v} f_0(\vec{v}) d^3v = 0$$

Calculation of the Current Density II

E-field means disturbance of the Fermi distribution by collisions:

$$f(\vec{v}) \neq f_0(\vec{v})$$

The calculation of the disturbed distribution function f(v) is the core of Boltzmann's transport theory!

The Boltzmann Equation

Descriptions of changes in f by collisions

$$\frac{df(\vec{r},\vec{v},t)}{dt} = \left(\frac{\partial f}{\partial t}\right)_{coll}$$

Formulation for charged particles

$$\frac{\partial f}{\partial t} + \vec{\nabla}_r f \underbrace{\frac{d\vec{r}}{dt}}_{v} + \vec{\nabla}_v f \underbrace{\frac{d\vec{v}}{dt}}_{a=\vec{F}/m=-\frac{e\vec{E}}{m}} = \left(\frac{\partial f}{\partial t}\right)_{coll}$$

$$\frac{\partial f}{\partial t} + \vec{v}\vec{\nabla}_r f - \frac{e\vec{E}}{m}\vec{\nabla}_v f = \left(\frac{\partial f}{\partial t}\right)_{coll}$$

Collisions and Relaxation

Ansatz for the collision term:

$$f(t) - f_0 = C \cdot e^{-t/\tau}$$

This yields:

$$\left(\frac{\partial f}{\partial t} \right)_{coll} = -\frac{f(t) - f_0}{\tau}$$

This means: after a disturbance of f_0 by a collision the disturbed function f exponentially approaches f_0 again.

The Disturbed Distribution Function f

Ansatz:

$$f = f_0 + A$$

A...Disturbance, independent on v

Insertion into Boltzmann equation:

$$\vec{v}\vec{\nabla}_r(\cancel{f}_0 + \cancel{A}) - \frac{eE}{m}\frac{\partial(f_0 + A)}{\partial v_x} = -\frac{1}{\tau}(\cancel{f}_0 + A - \cancel{f}_0)$$

$$A = \frac{eE}{m}\tau\frac{\partial f_0}{\partial v_x}$$

$$f = f_0 + \frac{eE}{m}\tau\frac{\partial f_0}{\partial v_x}$$

The derivate of f_0 to v has a profound influence on the calculation of the current density j!

Calculation of the Current Density III

Calculation of the current density with f insteadf of f_0:

$$f = f_0 + \frac{eE}{m}\tau\frac{\partial f_0}{\partial v_x}$$

Insertion into expression for j:

$$\vec{j}_e = -ne\vec{v} = -e\int \vec{v}\frac{dn}{V} = \left| dn = 2\cdot f(\vec{v})d\Phi \right| = -2e\left(\frac{m}{h}\right)^3\frac{1}{V}\int_{\vec{R},\vec{v}} \vec{v}f(\vec{v})d^3x\,d^3v$$

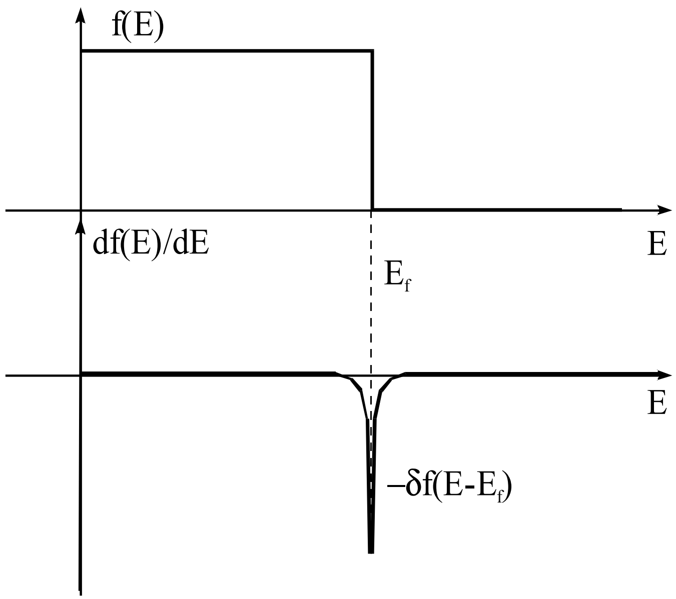
Calculation of j_x:

$$j_x = -2e\left(\frac{m}{h}\right)^3\frac{1}{V}\int_{\vec{R}} d^3x\underbrace{\int_{v} f_0(\vec{v})v_x d^3v}_{=0} - \frac{2e^2E}{m}\left(\frac{m}{h}\right)^3\tau\frac{1}{V}\int_{\vec{R}} d^3x\int_{v} v_x\frac{\partial f_0}{\partial v_x}d^3v =$$

$$= \left|\frac{1}{V}\cdot\int_{\vec{R}} d^3x = 1\right| = \underbrace{-2e^2E\frac{m^2}{h^3}\tau}_{C}\int_{\vec{v}} v_x\frac{\partial f_0}{\partial v_x}d^3v$$

Calculation of the Current Density IV

Solution of $\int_{\vec{v}} v_x \frac{\partial f_0}{\partial v_x} d^3v$ **:**



$$\int_{\vec{v}} v_x \frac{\partial f_0}{\partial v_x} d^3v = \left| d^3v = 4\pi v^2 dv \right| = \int_{\vec{v}} v_x \frac{\partial f_0}{\partial v_x} 4\pi v^2 dv =$$

$$\left| \frac{\partial f_0}{\partial v_x} = \frac{\partial f_0}{\partial E}\frac{\partial E}{\partial v_x} = \frac{\partial f_0}{\partial E} \cdot m v_x \right| = 4\pi m \int_{\vec{v}} v_x^2 \underbrace{\frac{\partial f_0}{\partial E}}_{-\delta(E-E_f)} v^2 dv$$

After some further transformations (appendix) one obtains:

$$j = \frac{8\pi e^2 \tau m^2 v_f^3}{3h^3} E = \sigma E$$

Comparison: Drude Model/Transport Theory

Drude:

$$\vec{j} = \frac{ne^2\tau}{2m_e}\vec{E} = \sigma \cdot \vec{E}$$

Boltzmann:

$$\vec{j} = \frac{8\pi e^2 \tau m_e{}^2 v_f^3}{3h^3}\vec{E} = \sigma\vec{E}$$

$$n = \frac{1}{V}\int dn =$$

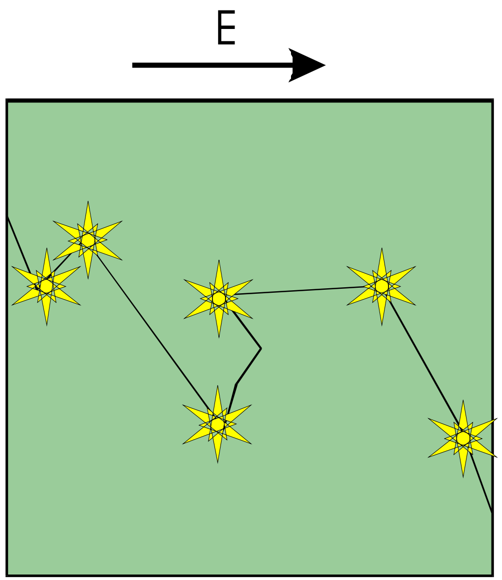
$$= \frac{1}{V}\int_{\vec{R},\vec{v}} 2f_0\left(\frac{m}{h}\right)^3 d^3x\,d^3v = \frac{8\pi}{3}\left(\frac{v_f m}{h}\right)^3$$

j_{Drude}=1/2$j_{Boltzmann}$

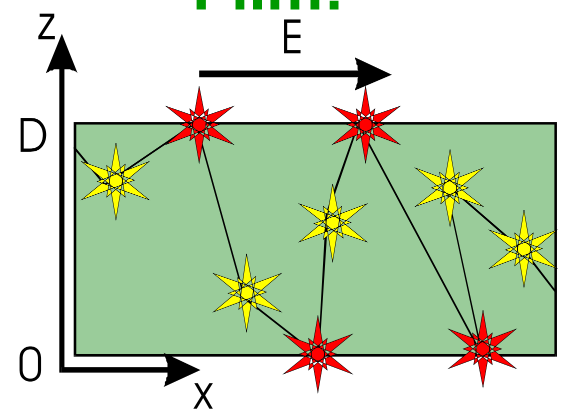
$$\vec{j} = \frac{ne^2\tau}{m_e}\vec{E} = \sigma \cdot \vec{E}$$

Transport Theory for Thin Films

Bulk:



Film:



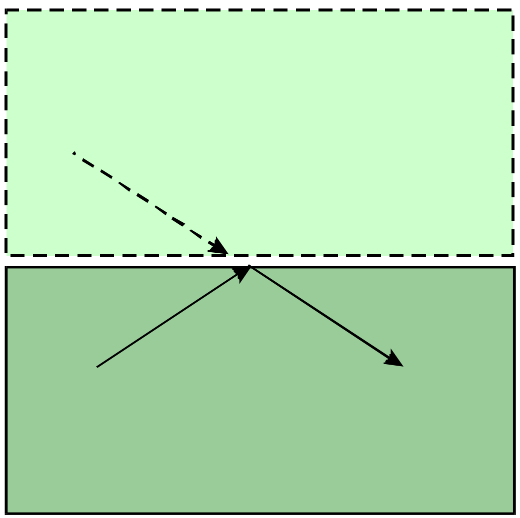
$$\frac{1}{\tau} = \frac{1}{\tau_G} + \frac{1}{\tau_K} + \frac{1}{\tau_V}$$

$$\frac{1}{\tau} = \frac{1}{\tau_G} + \frac{1}{\tau_K} + \frac{1}{\tau_V} + \frac{1}{\tau_I}$$

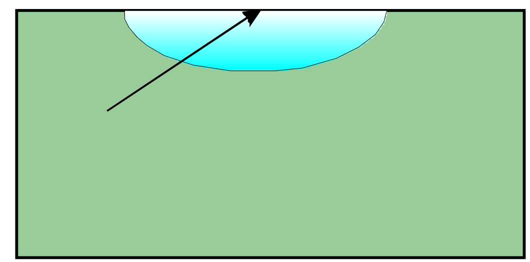
The Interfaces at z=0 and z=D are additional scattering centers for electrons!

Scattering at Interfaces

Specular:



Completely diffuse:



Specular reflexion does noct change the conductivity in comparison to the bulk!

The real case is a superposition of specular and diffuse scattering.

Current Density for Thin Films I

Ansatz:

$$f = f_0 + A$$

A...Disturbance, A=A(z)

Calculation analogous to previous yields (appendix):

$$j = \underbrace{-2e\left(\frac{m}{h}\right)^3 \tau \int \vec{v}\left(f_0 + \frac{eE}{m}\frac{\partial f_0}{\partial v_x}\right) d^3v}_{j_0} \underbrace{+2e\left(\frac{m}{h}\right)^3 \tau \int \vec{v}\,\frac{eE}{m}\frac{\partial f_0}{\partial v_x} \cdot e^{-\frac{z}{\tau v_z}} d^3v}_{\substack{\text{to solve for} \\ z=0 \rightarrow z=D}}$$

From this equation for j the average from z=0 to z=D has to be calculated to gain the conductivity of a film with the thickness D.

Current Density for Thin Films II

Total diffuse reflexion:

$$\frac{\sigma}{\sigma_0} = 1 - \frac{3}{8k} + \frac{3k}{4}\left(1 - \frac{k^2}{12}\right)\int_k^\infty \frac{e^{-x}}{x}dx + \left(\frac{3}{8k} - \frac{5}{8} - \frac{k}{16} + \frac{k^2}{16}\right)e^{-k}$$

Partially directed reflexion (fraction p):

$$\frac{\sigma}{\sigma_0} = 1 - \frac{3(1-p)}{8k} + \frac{3}{4k}(1-p)^2\sum_{n=0}^{\infty} p^{n-1}\left[E_1(kn)\left(k^2n^2 - \frac{k^4n^4}{12}\right) + e^{kn}\left(\frac{1}{2} - \frac{5kn}{6} - \frac{k^2n^2}{12} + \frac{k^3n^3}{12}\right)\right]$$

$$E_1(k) = \int_k^\infty \frac{e^{-x}}{x}dx$$

$k = D/\lambda_0$,
λ_0 = mean free pathn of electrons in metal
λ_0 = approx. 10 – 40 nm at room temperature

Conductivity of Thin Films I

Simplifications

Total diffuse reflexion:

k>>1

$$\frac{\sigma}{\sigma_0} = 1 - \frac{3}{8k}$$

0<k<<1

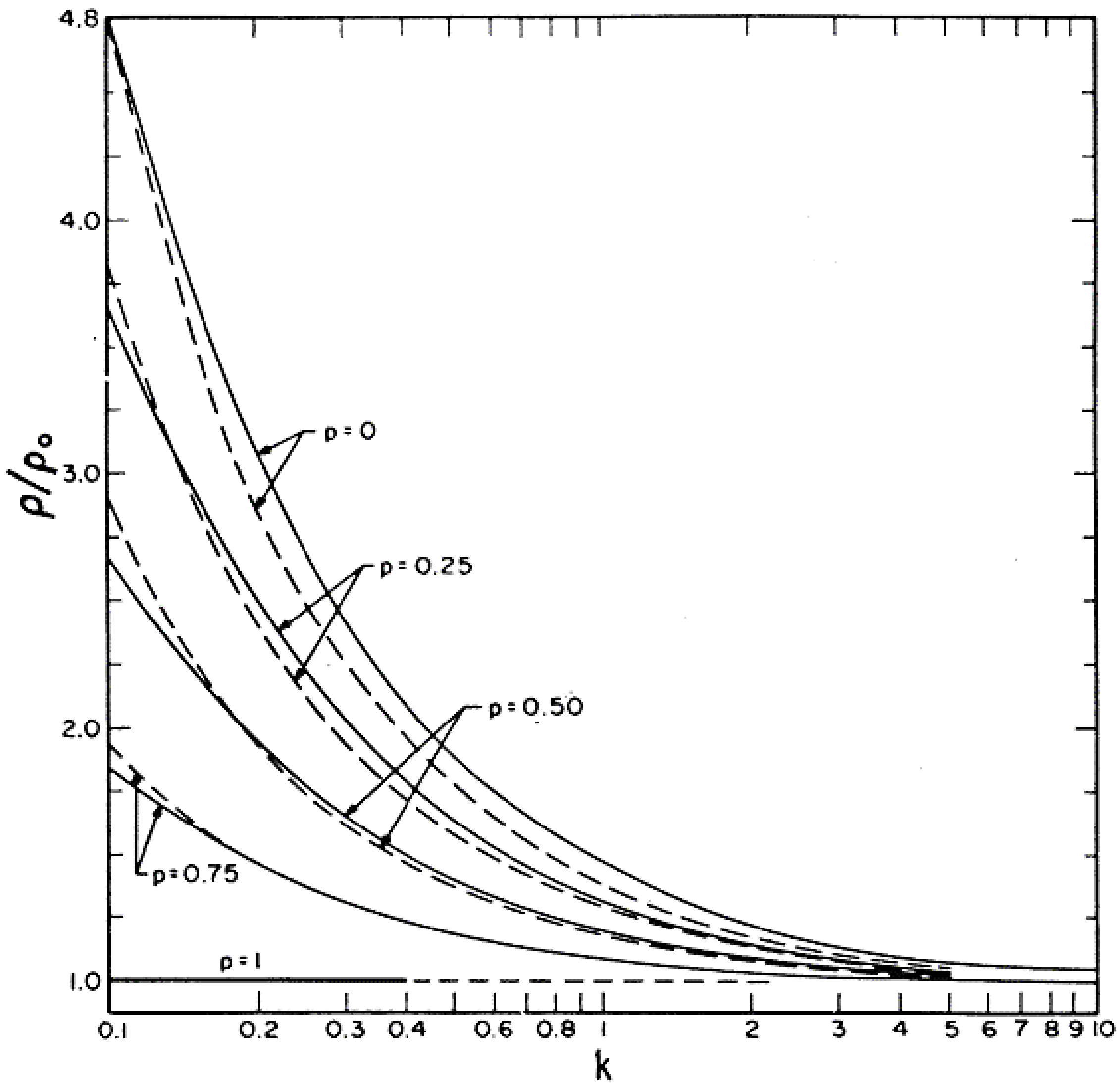
$$\frac{\sigma}{\sigma_0} = \frac{3k}{4} \ln \frac{1}{k}$$

Partially directed reflexion (fraction p):

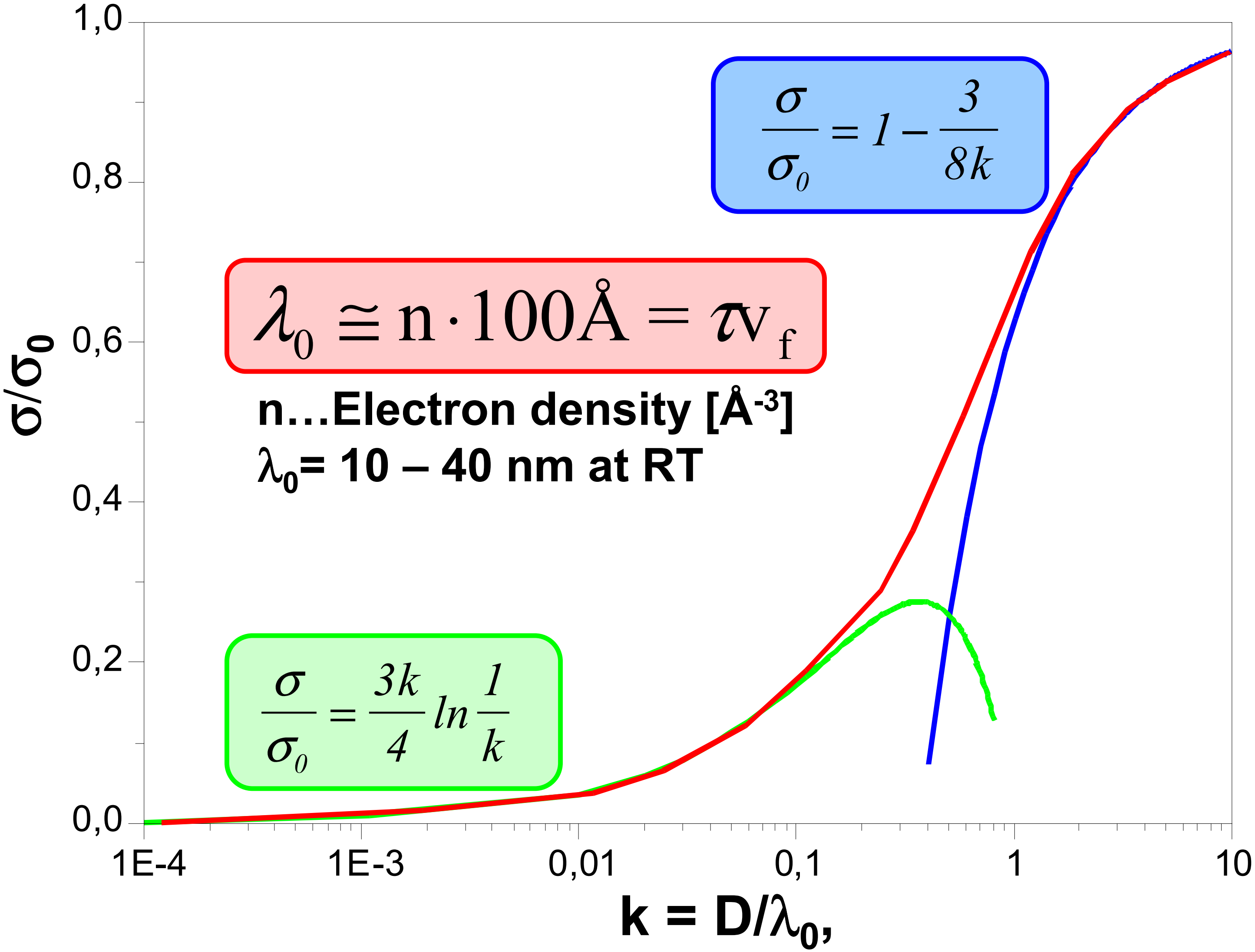
k>>1

$$\frac{\sigma}{\sigma_0} = 1 - \frac{3}{8k}(1-p)$$

Conductivity of Thin Films II



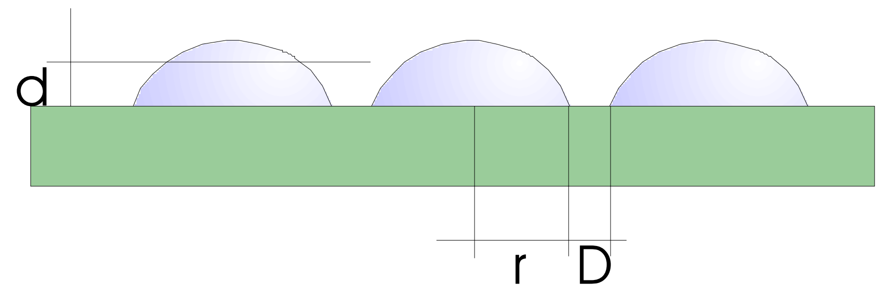
Conductivity Approximations



Real thin Film Systems

Ideal:

Real:



Experiment:

$$\sigma_{dis} << \sigma_{kont}$$

$$\sigma \propto e^{-A/k_B T}$$

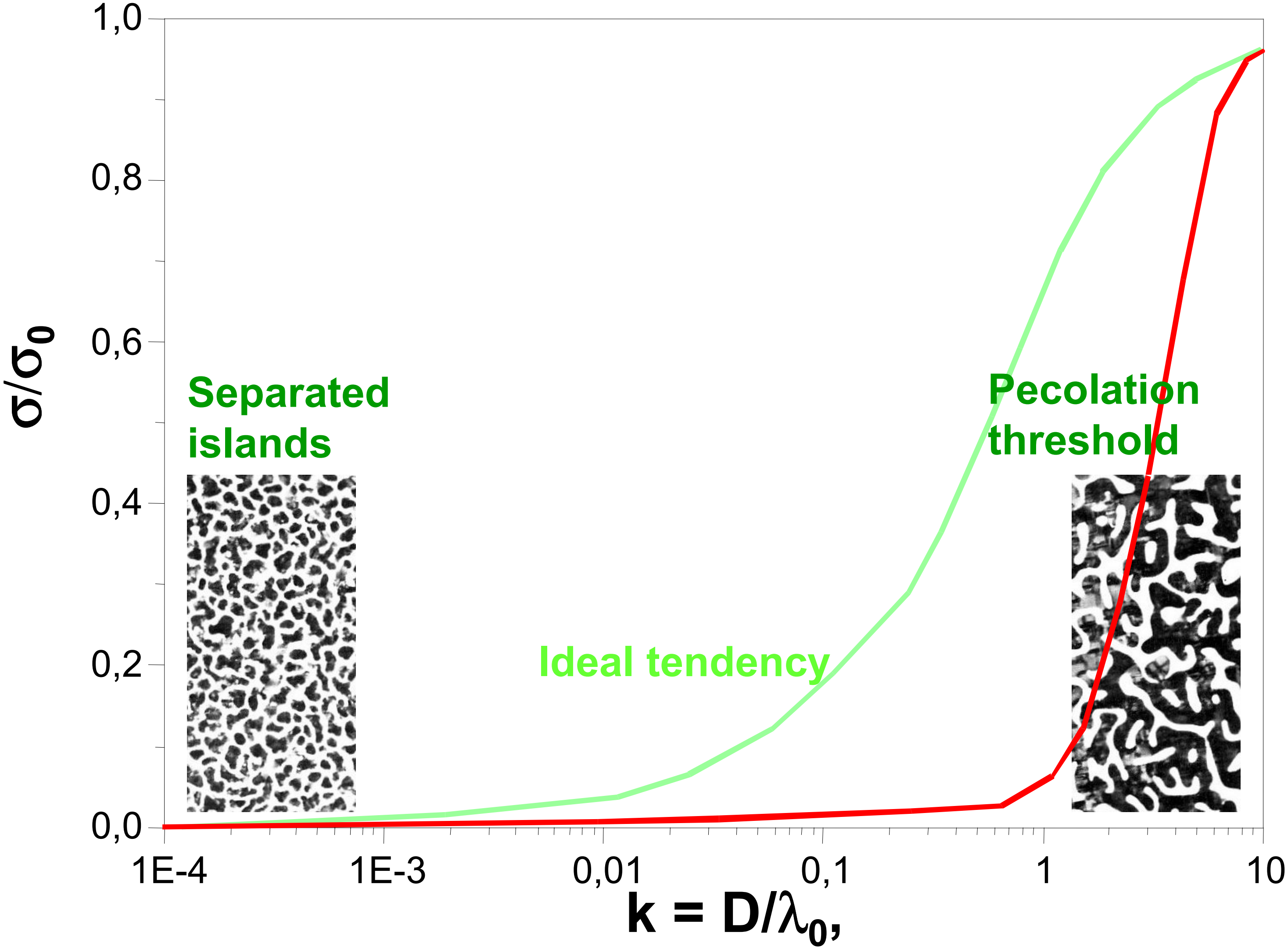
$$\sigma = \sigma(E)$$

$$\sigma = \sigma(r, D)$$

Justification:

Diskontinuity
Thermionic emission
Field emission
Tunnel effect

Conductivity and Film Thickness - Real



Application: Thin Film Resistors I

Region of resistivity:

$100\ \Omega_{\square} - 100\ \mathrm{M}\Omega_{\square}$

Covered by:

+ Film thickness variation
+ Choice of material

Voraussetzungen:

+ Low temperature coefficient
+ Low cost (bulk good!)

Application: Thin Film Resistors II