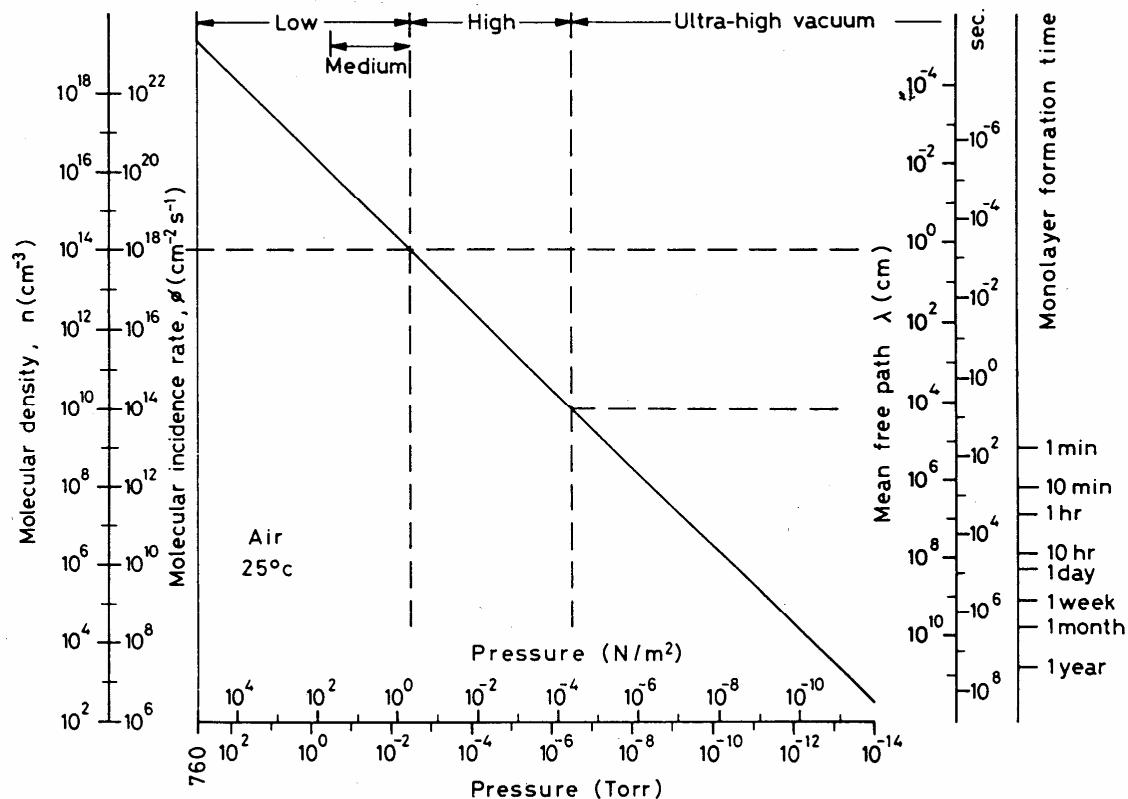


## Appendix

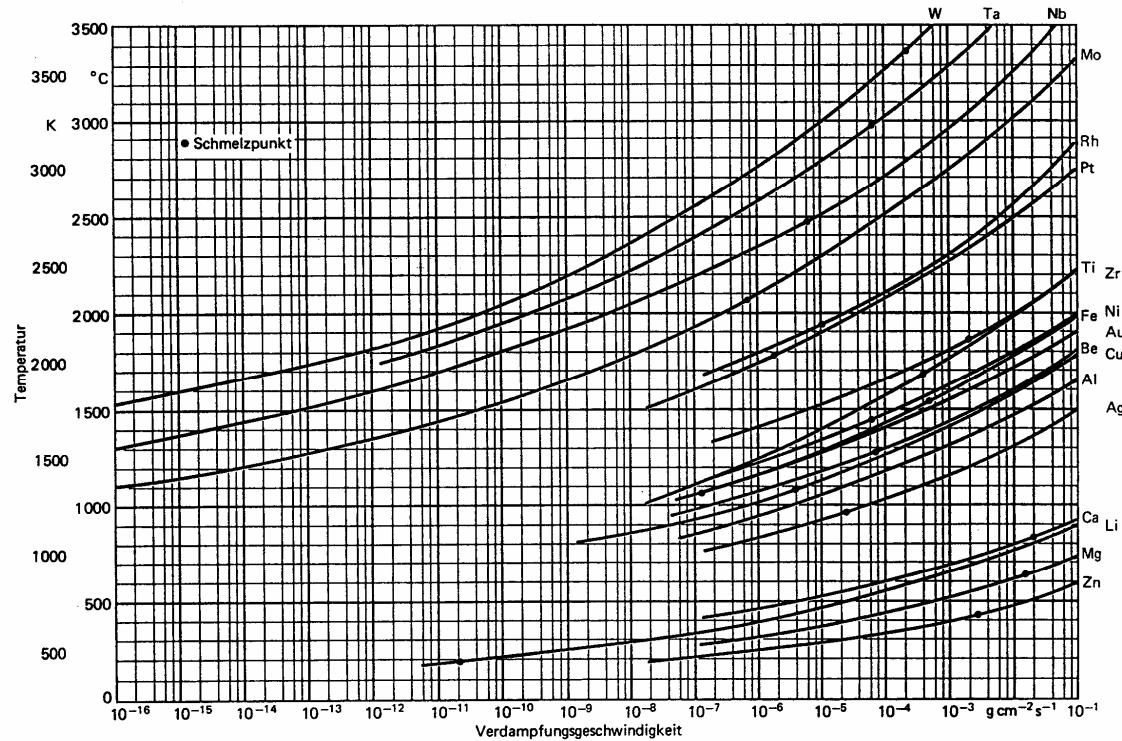
Vacuum Technique:



Time for the formation of a monolayer in dependence on the ambient pressure  
 Particle density  $n$ , impingement rate  $\Phi$ , mean free path  $\lambda$   
 [13, p. 2]

## Appendix

Evaporation Technique:



Evaporation velocity in high vacuum in dependence on the source temperature  
[3, p. 20]

## Appendix

Sputtering:

Target	Sputterausbeute $Y$ für $E_i$ in eV						$E_{\text{thres}}$	$E_0$
	200	600	1000	2000	5000	10 000		
	Atome/Ion						eV	eV/Atom
Ag	1,6	3,4				8,8	15	2,94
Al	0,35	1,2			2,0		13	3,33
Au	1,1	2,8	3,6	5,6	7,9		20	3,92
C	0,05	0,2					-	7,39
Co	0,6	1,4					25	4,40
Cr	0,7	1,3					22	4,11
Cu	1,1	2,3	3,2	4,3	5,5	6,6	17	3,50
Fe	0,5	1,3	1,4	2,0	2,5		20	4,13
Ge	0,5	1,2	1,5	2,0	3,0	3,98	25	-
Mo	0,4	0,9	1,1		1,5	2,2	24	6,88
Nb	0,25	0,65					25	-
Ni	0,7	1,5	2,1				21	4,45
Os	0,4	0,95					-	8,19
Pd	1,0	2,4					20	3,90
Pt	0,6	1,6					25	5,95
Re	0,4	0,9					35	8,06
Rh	0,55	1,5					24	5,76
Si	0,2	0,5	0,6	0,9	1,4		-	4,68
Ta	0,3	0,6			1,05		26	8,10
Th	0,3	0,7					24	5,97
Ti	0,2	0,6		1,1	1,7	2,1	20	4,86
U	0,35	1,0					23	5,00
W	0,3	0,6			1,1		33	8,80
Zr	0,3	0,75					22	6,34
Moleküle/Ion								
CdS (1010)	0,5	1,2						
GaAs (110)	0,4	0,9						
GaP (111)	0,4	1,0						
GaSb (111)	0,4	0,9	1,2					
InSb (110)	0,25	0,55						
PbTe (110)	0,6	1,40						
SiC (0001)		0,45						
SiO <sub>2</sub>			0,13	0,4				
Al <sub>2</sub> O <sub>3</sub>			0,04	0,11				

Sputter yield  $Y$  of different materials as a function of the energy  $E_i$  of impinging Ar-Ions, threshold energy  $E_{\text{thres}}$  and sublimation energy  $E_0$  [1, p. 98]

## Appendix

### Analytical Methods:

**Tabelle 8–7.** Analysemethoden und ihre Charakterisierungsart.

Methode	Abkürzungen	Anregung/ Detektion *)	Charakterisierungsart			elektronische Eigenschaften	Referenzen
			Chemische Analyse	Molekülkristall- strukturen	Mikroskopie		
Light Microscopy	LM	$h\nu \rightarrow h\nu$			×		[8–335]
Laser Scanning Microscopy	LSM	$h\nu \rightarrow h\nu$			×		[8–314; 8–416]
Ramanscattering	RS	$h\nu \rightarrow h\nu$		×			[8–395; 8–398 bis 8–402]
X-ray Photoelectron Spectrosc.	XPS	$h\nu \rightarrow e$	×				[8–340; 8–341; 8–434 bis 8–437]
Ultra Violet PS	UPS	$h\nu \rightarrow e$				×	[8–435; 8–436]
Laser Microprobe Mass Anal.	LAMMA	$h\nu \rightarrow i$	×				[8–438]
Photo Acoustic Spectroscopy	PAS	$h\nu \rightarrow ph$			×		[8–403]
Scanning Electron Microscopy	SEM	$e \rightarrow e$			×		[8–467; 8–430; 8–431; 8–432]
(Scan)Transmission Electr. Micr.	(S)TEM	$e \rightarrow e$		×			[8–466; 8–463 bis 8–466]
Electron Beam Induced Current	EBIC	$e \rightarrow e$			×	×	[8–467; 8–468; 8–469]
Voltage Contrast Microscopy	VCM	$e \rightarrow e$			×	×	[8–335]
Low Energy Electron Diffraction	LEED	$e \rightarrow e$		×			[8–357; 8–408; 8–409]
Reflective High EED	RHEED	$e \rightarrow e$		×			[8–359; 8–418; 8–419]
Auger Electron Spectroscopy	AES	$e \rightarrow e$	×		×		[8–340; 8–433; 8–434]
Electron Energy Loss Spectr.	EELS	$e \rightarrow e$	×	×			[8–357; 8–404 bis 8–407]
Electron Micro Probe	EMP	$e \rightarrow h\nu$	×				[8–439]
X-Ray Emission Spectroscopy	XES	$c \rightarrow h\nu$	×		×		[8–431; 8–432; 8–458; 8–459; 8–460]
Ion Scattering Spectroscopy	ISS	$i \rightarrow i$	×	(x)			[8–340; 8–410; 8–434]
Secondary Ion Mass Spectrosc.	SIMS	$i \rightarrow i$	×		×		[8–340; 8–346; 8–354; 8–440; 8–441; 8–442]
Rutherford Backscattering	RBS	$i \rightarrow i$	×	(x)			[8–454; 8–455; 8–456]
Secondary Neutral Mass Spectr.	SNMS	$i \rightarrow n$	×				[8–355]
Particle Induced X-Ray Emission	PIXE	$i \rightarrow h\nu$	✓				[8–356]
Field Ion Microscopy	FIM	$e \rightarrow i$	×		×		[8–340]
Scanning Tunneling Microscopy	STM	$e \rightarrow e$		×	×	(x)	[8–428; 8–429]
Scanning Acoustic Microscopy	SAM	$ph \rightarrow ph$			×		[8–416; 8–417]

\*)  $h\nu$  Photonen,  $ph$  Phononen,  $e$  Elektronen,  $i$  Ionen,  $n$  Neutralteilchen,  $c$  elektrisches Feld

[3, p. 342]

## Appendix

Calculation of the conductivity of thin films:

The starting point of all following considerations is the current density  $\vec{j}_e$ ,

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

Since  $e$  and  $\vec{v}$  are known, the electron density  $n$  has to be calculated:

$$dn = 2 \cdot f_0(E) \cdot d\Phi \quad d\Phi \dots \text{Phase space volume}$$

$$f_0(E) = \frac{1}{1 + e^{(E-E_f)/k_b T}} \dots \text{Fermi-distribution}$$

$$d\Phi = \frac{d^3x d^3p}{h^3} \dots \text{dimensionless, number of states in a phase space element of the size } d^3x d^3p$$

From quantum mechanics the number of possible states within a phase space element with the generalized coordinates  $(q, p)$ :  $\frac{d^3q d^3p}{h^3}$  is known: in a phase space element of the size  $h^3$  there can be only one state

### **a) Conductivity without electric field**

$$\begin{aligned} \vec{j}_e &= -e \int_{R, \vec{v}} \vec{v} \frac{dn}{V} = -2e \int_{R, \vec{v}} \vec{v} f_0(\vec{v}) \frac{d\Phi}{V} = \left| d\Phi = \left( \frac{m}{h} \right)^3 d^3x d^3v \right| = \\ &= -2e \left( \frac{m}{h} \right)^3 \frac{1}{V} \cdot \underbrace{\int_R d^3x \int_{\vec{v}} \vec{v} f_0(\vec{v}) d^3v}_{V} = -2e \left( \frac{m}{h} \right)^3 \int_{\vec{v}} \vec{v} f_0(\vec{v}) d^3v = 0 \end{aligned}$$

### **b) Conductivity with electric field in an infinite medium: Ohm's law**

Application of Boltzmann's transport theory:

General formulation of Boltzmann's equation:

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

i. e. changes in the distribution function are only due to collisions (extremely short interactions of the components of the system).

Total differential:

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

Special shape of Boltzmann's equation for the electric field:

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

Ansatz for the collision term determines the detailed solution of Boltzmann's equation:

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

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

Boundary conditions:  $\vec{E}$ -field in  $x$ -direction, homogeneous field strength.

Ansatz:  $f = f_0 + A$ ,  $A = A(E)$ ...distortion term, independent of  $\vec{v}$

$$\vec{v} \vec{\nabla}_r (f_0 + A) - \frac{eE}{m} \frac{\partial(f_0 + A)}{\partial v_x} = -\frac{I}{\tau} (f_0 + A - f_0), \text{ da}(\vec{\nabla}_r f_0 = 0)$$

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

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

The current density is again calculated by:

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

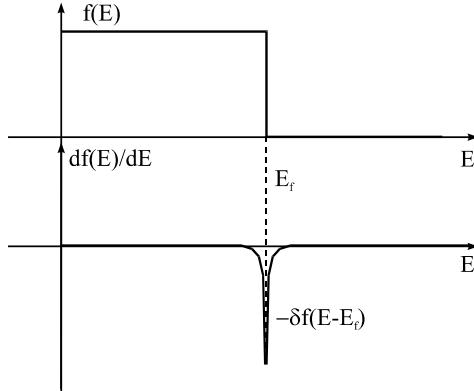
Calculation of one component of  $\vec{j}$ ,  $j_x$ :

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

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

$$= \left| \frac{I}{V} \cdot \int_{\tilde{R}} d^3x = I \right| = \underbrace{-2e^2 E \frac{m^2}{h^3} \tau \int_v v_x \frac{\partial f_0}{\partial v_x} d^3v}_C$$

In the above equation only the derivation  $\frac{\partial f_0}{\partial v_x}$  is unknown. It can be calculated by the known Fermi distribution and yields a Delta function (see sketch):



$$\begin{aligned}
 j_x &= C \int_{\vec{v}} v_x \frac{\partial f_0}{\partial v_x} d^3v = \left| d^3v = 4\pi v^2 dv \right| = C \cdot \int_{\vec{v}} v_x \frac{\partial f_0}{\partial v_x} 4\pi v^2 dv = \left| \frac{\partial f_0}{\partial v_x} = \frac{\partial f_0}{\partial E} \frac{\partial E}{\partial v_x} = \frac{\partial f_0}{\partial E} \cdot mv_x \right| = \\
 &= C \cdot 4\pi m \int_{\vec{v}} v_x^2 \underbrace{\frac{\partial f_0}{\partial E}}_{-\delta(E-E_f)} v^2 dv \\
 j_x &= -2e^2 E \tau \frac{m^2}{h^3} \cdot 4\pi m \int_{\vec{v}} v_x^2 \cdot [-\delta(E-E_f)] v^2 dv = 8\pi e^2 E \tau \left( \frac{m}{h} \right)^3 \cdot \underbrace{\int_{\vec{v}} v_x^2 \cdot [\delta(E-E_f)] v^2 dv}_{*}
 \end{aligned}$$

\* : Solution of the integral: solve analogous equations in y and z and the determines  $j_x + j_y + j_z$ :

$$\begin{aligned}
 * &= \int_{\vec{v}} [v_x^2 + v_y^2 + v_z^2] \delta(E - E_f) v^2 dv = \int_{\vec{v}} v^4 \delta(E - E_f) dv = \left| dv = \frac{dE}{mv} \right| = \int_E m^{-1} v^3 \delta(E - E_f) dE = \\
 &= \int_E m^{-1} \left( \frac{2E}{m} \right)^{3/2} \delta(E - E_f) dE = m^{-1} \left( \frac{2E_f}{m} \right)^{3/2} = m^{-1} v_f^3
 \end{aligned}$$

$$j_x = \frac{1}{3} (j_x + j_y + j_z) = 8\pi e^2 E \tau \frac{m^2}{h^3} \cdot v_f^3$$

Arbitrary co ordinate system:

$$\begin{aligned}
 j &= \frac{1}{3} j_x = \frac{8\pi e^2 E \tau m^2 v_f^3}{3h^3} E = \sigma E \\
 \sigma &= \frac{8\pi e^2 E \tau m^2 v_f^3}{3h^3} = \frac{ne^2}{m} \tau, \text{ weil} \\
 n &= \frac{1}{V} \int dn = \frac{1}{V} \int_{R,\vec{v}} 2f_0 \left( \frac{m}{h} \right)^3 d^3x d^3v = \frac{8\pi}{3} \left( \frac{v_f m}{h} \right)^3
 \end{aligned}$$

### c) Conductivity of thin films: Fuchs-Sondheimer-equation

Ansatz:  $f = f_0 + A$ ,  $A=A(E, z)$ ...distortion term, independent of  $\vec{v}$ , but now dependent on the position within the film

Possible boundary conditions:

- \* Specular reflection at the film interfaces: no difference to the bulk

- \* Diffuse reflection at the film interfaces:

Ansatz for  $f(v, E, z)$ :  $f = f_0 + A(E, z)$

Boundary condition for diffuse reflection:  $f(z=0)=f_0$

$$f(z=0) = f_0 = \underbrace{\frac{eE\tau}{m} \frac{\partial f_0}{\partial v_x}}_{A(z=0)} (1 + K) + f_0$$

$$\Rightarrow K = -1$$

$$j = -2e \left( \frac{m}{h} \right)^3 \tau \int \vec{v} \left( f_0 + \underbrace{\frac{eE}{m} \frac{\partial f_0}{\partial v_x}}_{J_0} \right) d^3v + 2e \left( \frac{m}{h} \right)^3 \tau \int \vec{v} \underbrace{\frac{eE}{m} \frac{\partial f_0}{\partial v_x} \cdot e^{-\frac{z}{\tau v_z}} d^3v}_{I \text{ zu lösen für } z=0 \rightarrow z=D}$$

For solving I the average from  $z = 0$  to  $z=D$  has to be calculated, then  $\Rightarrow$  script. 4.57

## Appendix

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