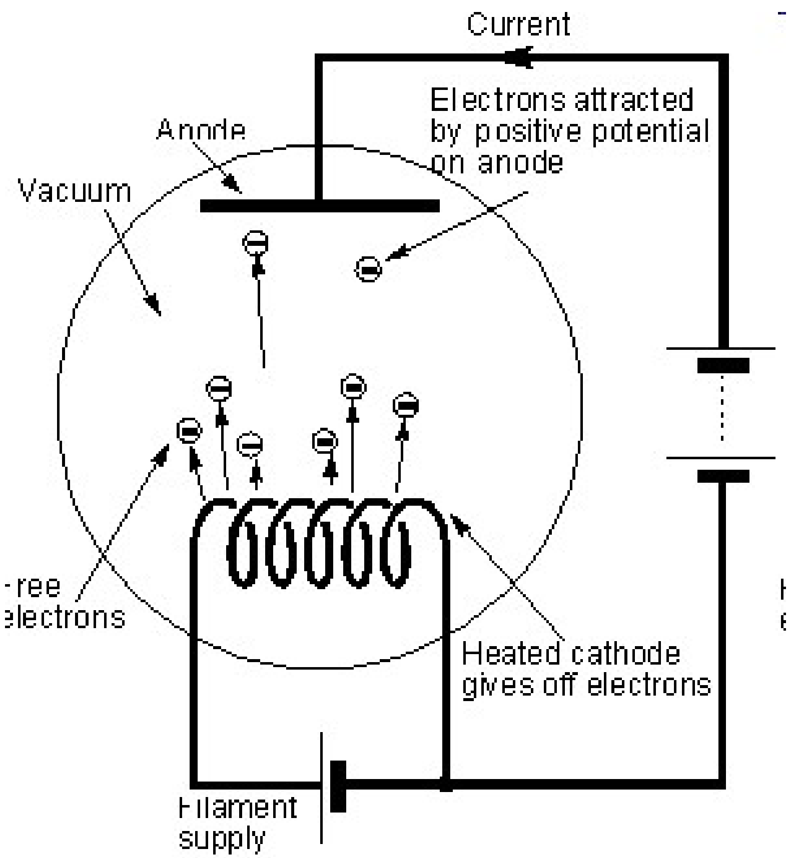
Thermal conductivity, Crystal physics

Ballistic motion



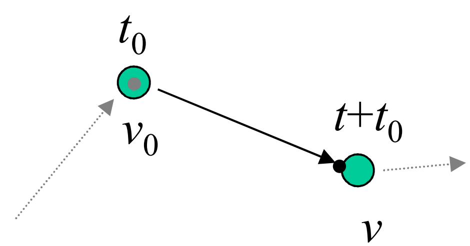
diode

Diffusive transport

$$\vec{F} = -e\vec{E} = m^*\vec{a} = m^*\frac{d\vec{v}}{dt}$$

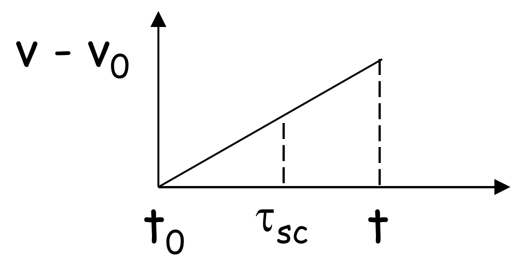
$$\vec{v} = \vec{v}_0 - \frac{e\vec{E}}{m^*}(t - t_0)$$

time between two collisions



$\langle v_0 \rangle = 0$

$\langle t - t_0 \rangle = \tau_{sc}$ < average time between scattering events



$$\vec{v}_d = \frac{-e\vec{E}\tau_{sc}}{m^*} = \frac{-e\vec{E}\ell}{m^* v_F}$$

drift velocity: $\vec{v}_d = -\mu\vec{E}$

Ohm's law: $\vec{j} = -ne\vec{v}_d = ne\mu\vec{E} = \sigma\vec{E}$

Matthiessen's rule

$$\frac{1}{\tau_{sc}} = \frac{1}{\tau_{sc,lattice}} + \frac{1}{\tau_{sc,impurity}}$$

mostly temperature independent

phonons, temperature dependent

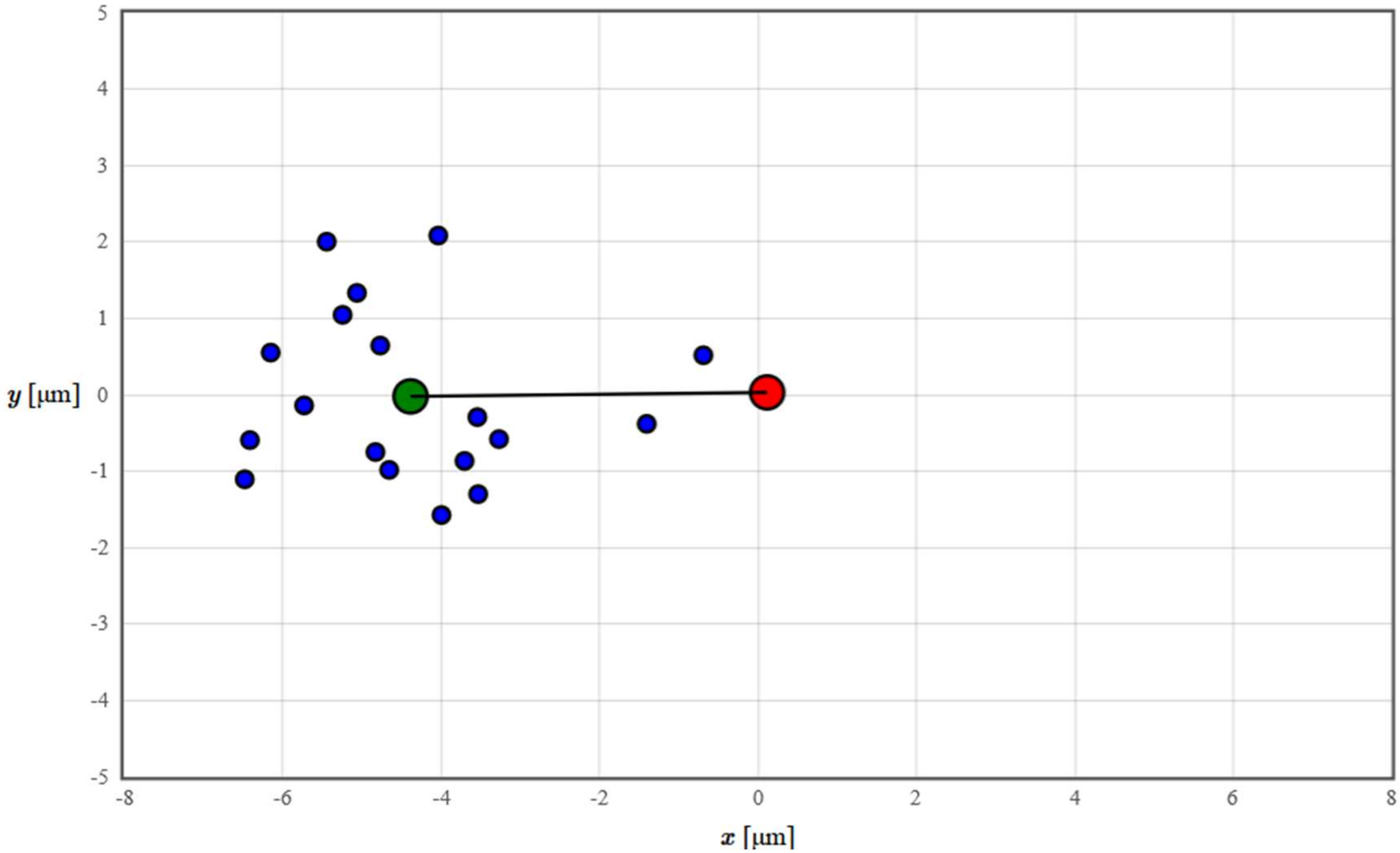
$$\frac{1}{\mu} = \frac{1}{\mu_{lattice}} + \frac{1}{\mu_{impurity}}$$

Waves or Particles

Scattering between Bloch states can be calculated by Fermi's golden rule.

The particle picture is not rigorously correct.

Drift and Diffusion

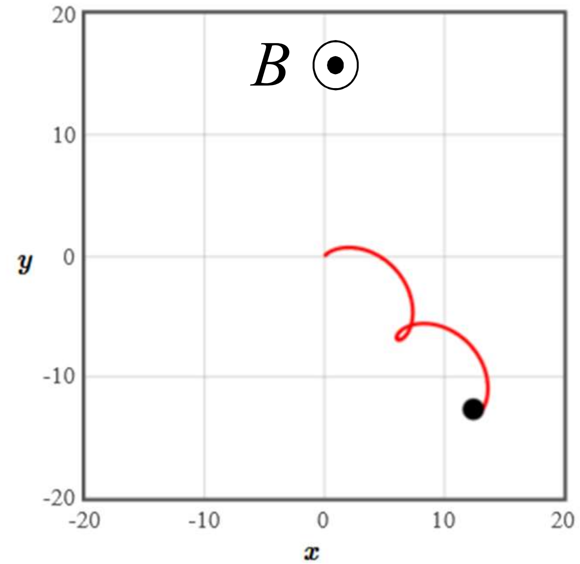


http://lampx.tugraz.at/~hadley/ss2/transport/drude.php

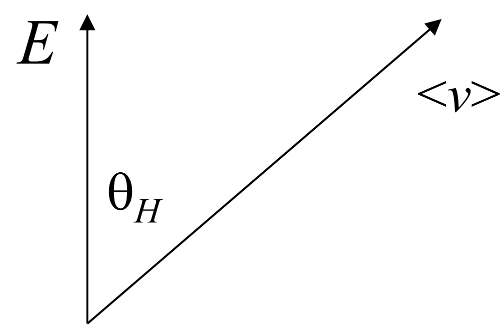
Crossed *E* and *B* fields

Ballistic transport

$$\vec{F} = m\vec{a} = -e\left(\vec{E} + \vec{v} \times \vec{B}\right)$$



Diffusive transport



Hall angle: $$\theta_H = \tan^{-1}\left(-\frac{eB_z\tau_{sc}}{m}\right)$$

Magnetic field (diffusive regime)

$$\vec{F} = m\vec{a} = -e\vec{E} = m\frac{\vec{v}_d}{\tau_{\mathrm{sc}}} \qquad -\frac{e\tau_{\mathrm{sc}}}{m}\vec{E} = \vec{v}_d$$

$$\vec{F} = m\vec{a} = -e\left(\vec{E} + \vec{v}\times\vec{B}\right) = m\frac{\vec{v}_d}{\tau_{\mathrm{sc}}}$$

If B is in the z-direction, the three components of the force are

$$-e\left(E_x + v_{dy}B_z\right) = m\frac{v_{dx}}{\tau_{\mathrm{sc}}}$$

$$-e\left(E_y - v_{dx}B_z\right) = m\frac{v_{dy}}{\tau_{\mathrm{sc}}}$$

$$-e\left(E_z\right) = m\frac{v_{dz}}{\tau_{\mathrm{sc}}}$$

Magnetic field (diffusive regime)

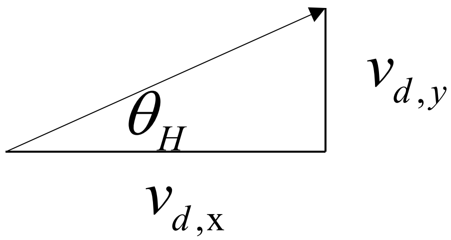
$$v_{d,x} = -\frac{eE_x\tau_{sc}}{m} - \frac{eB_z}{m}\tau_{sc}v_{d,y}$$

$$v_{d,y} = -\frac{eE_y\tau_{sc}}{m} + \frac{eB_z}{m}\tau_{sc}v_{d,x}$$

$$v_{d,z} = -\frac{eE_z\tau_{sc}}{m}$$

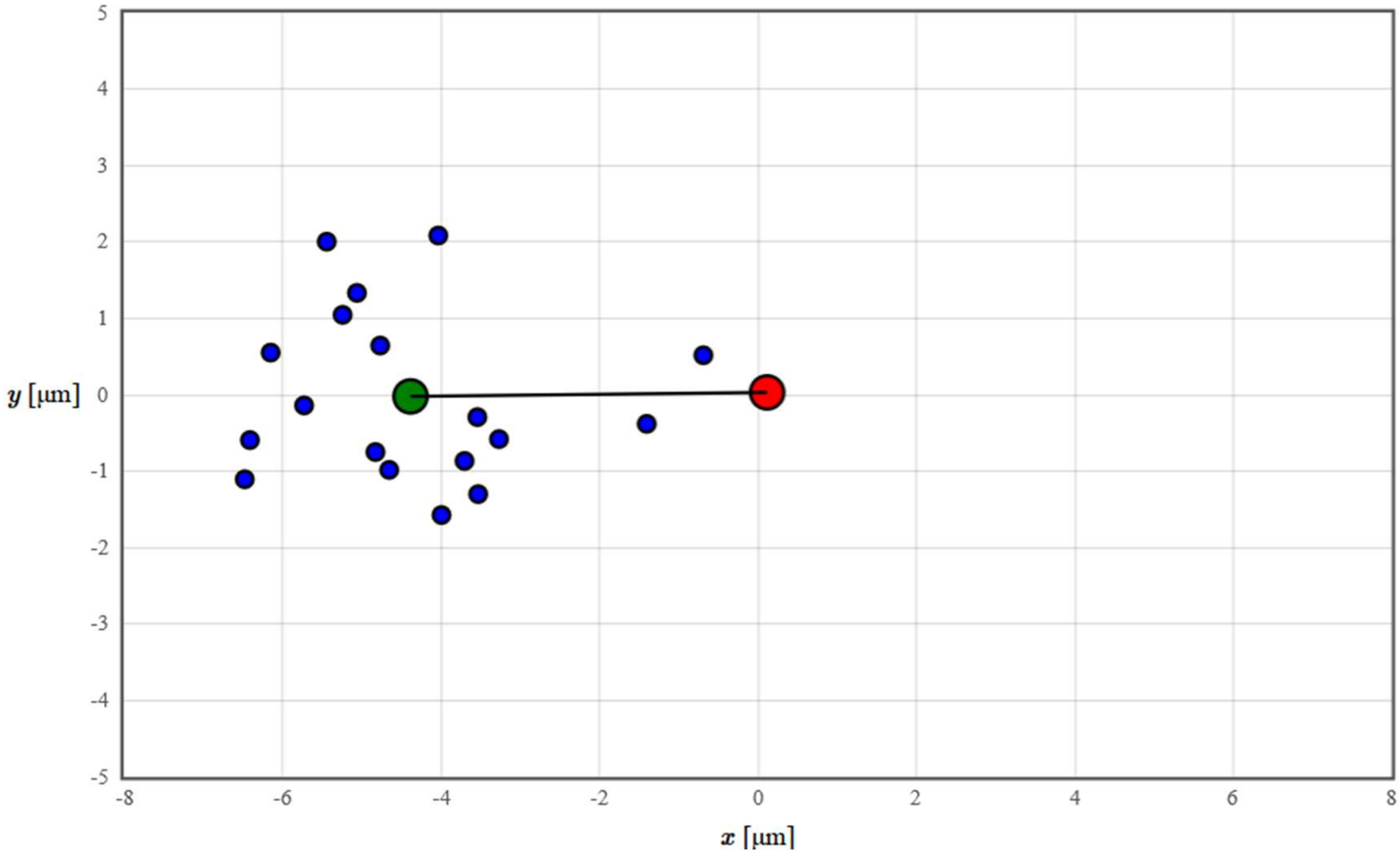
If $E_y = 0,\, E_z = 0$

$$v_{d,y} = -\frac{eB_z}{m}\tau_{sc}v_{d,x}$$



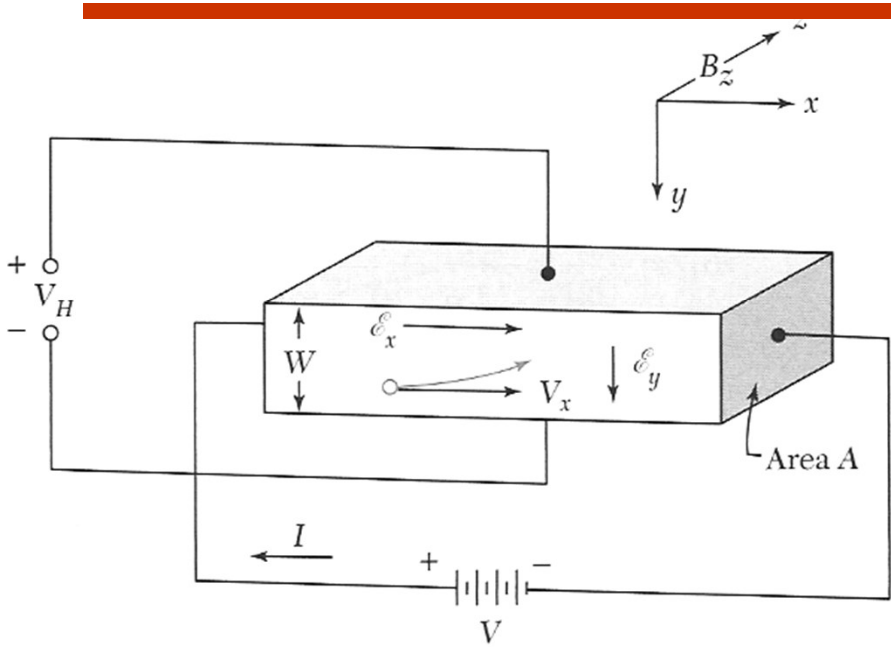
$$\tan\theta_H = -\frac{eB_z}{m}\tau_{sc}$$

Drift and Diffusion



http://lampx.tugraz.at/~hadley/ss2/transport/drude.php

The Hall Effect (diffusive regime)



$$v_{d,x} = -\frac{eE_x\tau_{sc}}{m} - \frac{eB_z}{m}\tau_{sc}v_{d,y}$$

$$v_{d,y} = -\frac{eE_y\tau_{sc}}{m} + \frac{eB_z}{m}\tau_{sc}v_{d,x}$$

$$v_{d,z} = -\frac{eE_z\tau_{sc}}{m}$$

If $v_{d,y} = 0$,

$E_y = v_{d,x}B_z = V_H/W = R_H j_x B_z$ $\quad$ V_H = Hall voltage, R_H = Hall Constant

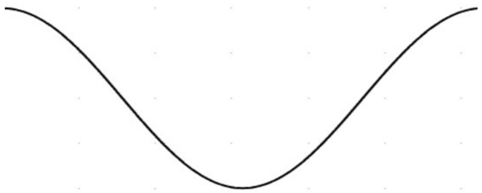
$j_x = - nev_{d,x}$

$$\boxed{R_H = E_y/j_xB_z = -1/ne}$$

Metal	Method	Experimental R_H, in 10^{-24} CGS units	Assumed carriers per atom	Calculated $-1/nec$, in 10^{-24} CGS units
Li	conv.	-1.89	1 electron	-1.48
Na	helicon	-2.619	1 electron	-2.603
	conv.	-2.3		
K	helicon	-4.946	1 electron	-4.944
	conv.	-4.7		
Rb	conv.	-5.6	1 electron	-6.04
Cu	conv.	-0.6	1 electron	-0.82
Ag	conv.	-1.0	1 electron	-1.19
Au	conv.	-0.8	1 electron	-1.18
Be	conv.	$+2.7$	—	—
Mg	conv.	-0.92	—	—
Al	helicon	$+1.136$	1 hole	$+1.135$
In	helicon	$+1.774$	1 hole	$+1.780$
As	conv.	$+50.$	—	—
Sb	conv.	$-22.$	—	—
Bi	conv.	$-6000.$	—	—

Kittel

Einstein relation



$$n(x) = A\exp\left(\frac{-U_{pot}(x)}{k_B T}\right)$$ Boltzmann factor

$$\vec{F} = -\nabla U_{pot} = -e\vec{E}$$

In equilibrium, drift = diffusion

$$en\mu\vec{E} + eD\nabla n = 0$$

$$\nabla n = -\frac{1}{k_B T} A\exp\left(\frac{-U_{pot}}{k_B T}\right)\nabla U_{pot} = -\frac{n}{k_B T}\nabla U_{pot} = \frac{-en\vec{E}}{k_B T}$$

$$en\mu\vec{E} - e^2 D\frac{n\vec{E}}{k_B T} = 0$$

$$\boxed{D = \frac{\mu k_B T}{e}}$$

Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen, A. Einstein (1905).

Thermal conductivity

$$\vec{j}_U = \bar{E}\vec{j}$$

Average particle energy

$$u = \bar{E}n$$

internal energy density

$$\vec{j}_U = -\bar{E}D\nabla n = -D\nabla u$$

$$\vec{j}_U = -D\frac{du}{dT}\nabla T = -Dc_v\nabla T$$

$$\vec{j}_U = -K\nabla T$$

Thermal conductivity

$$K = Dc_v$$

$$K \to 0 \quad \text{as} \quad T \to 0$$

Wiedemann - Franz law

$$\frac{K}{\sigma} = \frac{Dc_v}{ne\mu}$$

Einstein relation: $$D = \frac{\mu k_B T}{e}$$

Dulong - Petit: $$c_v = 3nk_B$$

$$\frac{K}{\sigma} = \frac{3k_B^2}{e^2} T$$

Wiedemann Franz law $$L = \frac{K_{el}}{\sigma T} = 2.22 \times 10^{-8} \quad \mathrm{W}\ \Omega / \mathrm{K}^2$$

Lorentz number

Lorenz number

$$L = \frac{K_{el}}{\sigma T} = 2.22\times 10^{-8} \qquad \mathrm{W\,\Omega / K^2}$$

Table 5 Experimental Lorenz numbers

	$L \times 10^8$ watt-ohm/deg^2			$L \times 10^8$ watt-ohm/deg^2	
Metal	0°C	100°C	Metal	0°C	100°C
Ag	2.31	2.37	Pb	2.47	2.56
Au	2.35	2.40	Pt	2.51	2.60
Cd	2.42	2.43	Su	2.52	2.49
Cu	2.23	2.33	W	3.04	3.20
Mo	2.61	2.79	Zn	2.31	2.33

At low temperatures the classical predictions for the thermal and electrical conductivities are too high but their ratio is correct. Only the electrons within $k_B T$ of the Fermi surface contribute.

Summary

Drift: $\vec{v}_d = -\mu \vec{E}$

Ohm's law: $\vec{j} = -ne\vec{v}_d = ne\mu\vec{E} = \sigma\vec{E}$

Diffusion: $\frac{dn}{dt} = -D\nabla^2 n$

Fick's law: $\vec{j} = -D\nabla n$

Continuity equation $\frac{dn}{dt} = \nabla \cdot \vec{j}$

Hall effect: $\tan\theta_H = -\frac{eB_z}{m}\tau_{sc}$

$R_H = E_y/j_x B_z = -1/ne$

Einstein relation: $D = \frac{\mu k_B T}{e}$

Wiedemann Franz law: $L = \frac{K_{el}}{\sigma T} = 2.22 \times 10^{-8}$ $\mathrm{W\ \Omega / K^2}$

Crystal Physics

Crystal physics explains what effects the symmetries of the crystal have on observable quantities.

An Introduction to Crystal Physics Ervin Hartmann
http://ww1.iucr.org/comm/cteach/pamphlets/18/index.html

International Tables for Crystallography
http://it.iucr.org/

Kittel chapter 3: elastic strain

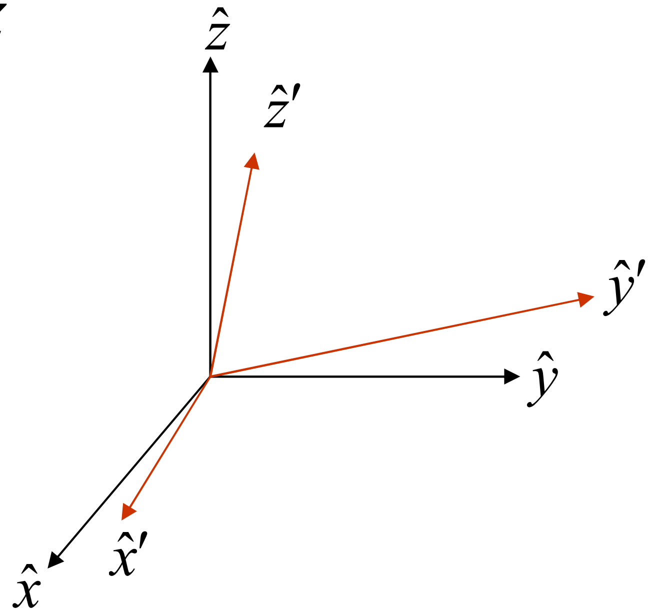
Strain

A distortion of a material is described by the strain matrix

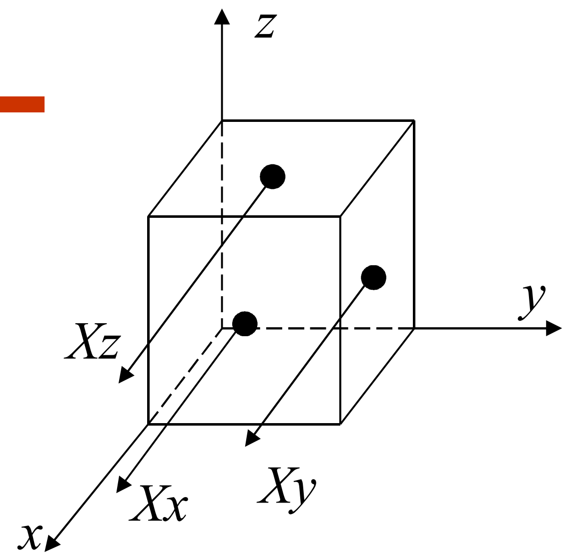
$$x' = (1+\varepsilon_{xx})\hat{x} + \varepsilon_{xy}\hat{y} + \varepsilon_{xz}\hat{z}$$

$$y' = \varepsilon_{yx}\hat{x} + (1+\varepsilon_{yy})\hat{y} + \varepsilon_{yz}\hat{z}$$

$$z' = \varepsilon_{zx}\hat{x} + \varepsilon_{zy}\hat{y} + (1+\varepsilon_{zz})\hat{z}$$



Stress



9 forces describe the stress

Xx, Xy, Xz, Yx, Yy, Yz, Zx, Zy, Zz

Xx is a force applied in the *x*-direction to the plane normal to *x*

Xy is a sheer force applied in the *x*-direction to the plane normal to *y*

stress tensor:

$$\sigma = \begin{bmatrix} \frac{X_x}{A_x} & \frac{X_y}{A_y} & \frac{X_z}{A_z} \\ \frac{Y_x}{A_x} & \frac{Y_y}{A_y} & \frac{Y_z}{A_z} \\ \frac{Z_x}{A_x} & \frac{Z_y}{A_y} & \frac{Z_z}{A_z} \end{bmatrix}$$

Stress is force/m^2

Stress and Strain

$$\varepsilon_{ij} = s_{ijkl}\sigma_{kl}$$

The stress - strain relationship is described by a rank 4 stiffness tensor. The inverse of the stiffness tensor is the compliance tensor.

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$$

Einstein convention: sum over repeated indices.

$$\varepsilon_{xx} = s_{xxxx}\sigma_{xx} + s_{xxxy}\sigma_{xy} + s_{xxxz}\sigma_{xz} + s_{xxyx}\sigma_{yx} + s_{xxyy}\sigma_{yy}$$
$$+ s_{xxyz}\sigma_{yz} + s_{xxzx}\sigma_{zx} + s_{xxzy}\sigma_{zy} + s_{xxzz}\sigma_{zz}$$

Statistical Physics

Microcannonical Ensemble: Internal energy is expressed in terms of extrinsic quantities $U(S, M, P, \varepsilon, N, V)$.

$$dU = \frac{\partial U}{\partial S} dS + \frac{\partial U}{\partial \varepsilon_{ij}} d\varepsilon_{ij} + \frac{\partial U}{\partial P_k} dP_K + \frac{\partial U}{\partial M_l} dM_l$$

$$dU = TdS + \sigma_{ij} d\varepsilon_{ij} + E_k dP_K + H_l dM_l$$

The normal modes must be solved for in the presence of electric and magnetic fields (Advanced Solid State Physics course).

Internal energy in an electric field

In an electric field, if the dipole moment is changed, the change of the energy is,

$$\Delta U = \vec{E} \cdot \Delta \vec{P}$$

Using Einstein notation

$$dU = E_k dP_k$$

This is part of the total derivative of U

$$dU = TdS + \sigma_{ij} d\varepsilon_{ij} + E_k dP_K + H_l dM_l$$

Statistical Physics

Microcannonical Ensemble: Internal energy is expressed in terms of extrinsic quantities $U(S, M, P, \varepsilon, N, V)$. $\varepsilon_{ij} \Rightarrow V\varepsilon_{ij}$

$$dU = \frac{\partial U}{\partial S} dS + \frac{\partial U}{\partial \varepsilon_{ij}} d\varepsilon_{ij} + \frac{\partial U}{\partial P_k} dP_K + \frac{\partial U}{\partial M_l} dM_l$$

$$dU = TdS + \sigma_{ij} d\varepsilon_{ij} + E_k dP_K + H_l dM_l$$

Cannonical ensemble: At constant temperature, make a Legendre transformation to the Helmholtz free energy.

$F = U - TS$

$F(V, T, N, M, P, \varepsilon)$

Make a Legendre transformation to the Gibbs potential $G(T, H, E, \sigma)$

$$G = U - TS - \sigma_{ij}\varepsilon_{ij} - E_k P_K - H_l M_l$$

Gibbs free energy

$$G = U - TS - \sigma_{ij}\varepsilon_{ij} - E_k P_K - H_l M_l$$

$$dG = dU - TdS - SdT - \sigma_{ij} d\varepsilon_{ij} - \varepsilon_{ij} d\sigma_{ij} - E_k dP_k - P_k dE_k - H_l dM_l - M_l dH_l$$

$$dU = TdS + \sigma_{ij} d\varepsilon_{ij} + E_k dP_K + H_l dM_l$$

$$dG = -SdT - \varepsilon_{ij} d\sigma_{ij} - P_k dE_k - M_l dH_l$$

total derivative: $dG = \left(\frac{\partial G}{\partial T}\right) dT + \left(\frac{\partial G}{\partial \sigma_{ij}}\right) d\sigma_{ij} + \left(\frac{\partial G}{\partial E_k}\right) dE_k + \left(\frac{\partial G}{\partial H_l}\right) dH_l$

$$\left(\frac{\partial G}{\partial \sigma_{ij}}\right) = -\varepsilon_{ij} \qquad \left(\frac{\partial G}{\partial E_k}\right) = -P_k$$

$$\left(\frac{\partial G}{\partial H_l}\right) = -M_l \qquad \left(\frac{\partial G}{\partial T}\right) = -S$$

$$d\varepsilon_{ij} = \underset{1}{\left(\frac{\partial \varepsilon_{ij}}{\partial \sigma_{kl}}\right)} d\sigma_{kl} + \underset{2}{\left(\frac{\partial \varepsilon_{ij}}{\partial E_k}\right)} dE_k + \underset{3}{\left(\frac{\partial \varepsilon_{ij}}{\partial H_l}\right)} dH_l + \underset{4}{\left(\frac{\partial \varepsilon_{ij}}{\partial T}\right)} dT$$

$$dP_i = \underset{5}{\left(\frac{\partial P_i}{\partial \sigma_{kl}}\right)} d\sigma_{kl} + \underset{6}{\left(\frac{\partial P_i}{\partial E_k}\right)} dE_k + \underset{7}{\left(\frac{\partial P_i}{\partial H_l}\right)} dH_l + \underset{8}{\left(\frac{\partial P_i}{\partial T}\right)} dT$$

$$dM_i = \underset{9}{\left(\frac{\partial M_i}{\partial \sigma_{kl}}\right)} d\sigma_{kl} + \underset{10}{\left(\frac{\partial M_i}{\partial E_k}\right)} dE_k + \underset{11}{\left(\frac{\partial M_i}{\partial H_l}\right)} dH_l + \underset{12}{\left(\frac{\partial M_i}{\partial T}\right)} dT$$

$$dS = \underset{13}{\left(\frac{\partial S}{\partial \sigma_{kl}}\right)} d\sigma_{kl} + \underset{14}{\left(\frac{\partial S}{\partial E_k}\right)} dE_k + \underset{15}{\left(\frac{\partial S}{\partial H_l}\right)} dH_l + \underset{16}{\left(\frac{\partial S}{\partial T}\right)} dT$$

1. Elastic deformation.
2. Reciprocal (or converse) piezo-electric effect.
3. Reciprocal (or converse) piezo-magnetic effect.
4. Thermal dilatation.
5. Piezo-electric effect.
6. Electric polarization.
7. Magneto-electric polarization.
8. Pyroelectricity.
9. Piezo-magnetic effect.
10. Reciprocal (or converse) magneto-electric polarization.
11. Magnetic polarization.
12. Pyromagnetism.
13. Piezo-caloric effect.
14. Electro-caloric effect.
15. Magneto-caloric effect.
16. Heat transmission.