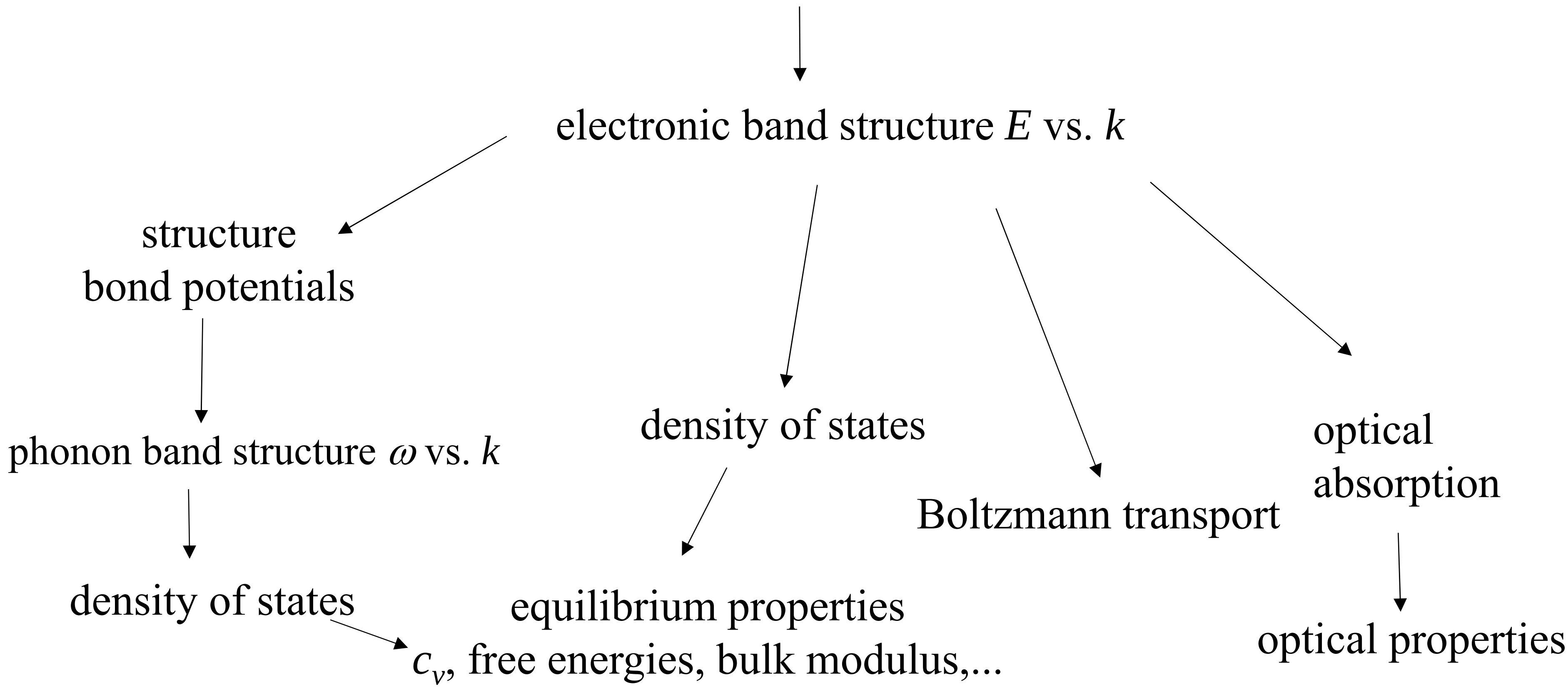
Crystal Physics

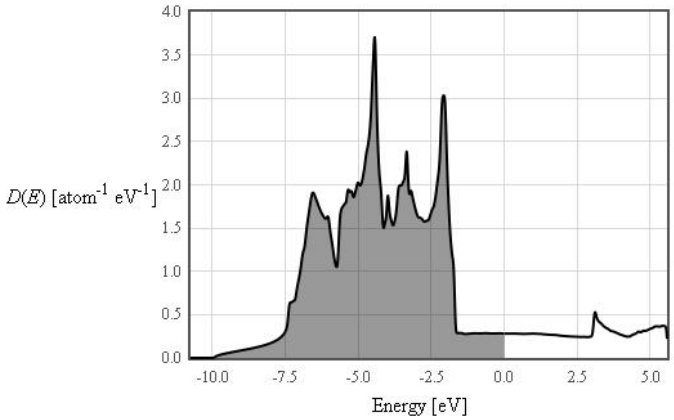
The properties of solids

$$H = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_A \frac{\hbar^2}{2m_A}\nabla_A^2 - \sum_{i,A}\frac{Z_A e^2}{4\pi\varepsilon_0 r_{iA}} + \sum_{i<j}\frac{e^2}{4\pi\varepsilon_0 r_{ij}} + \sum_{A<B}\frac{Z_A Z_B e^2}{4\pi\varepsilon_0 r_{AB}}$$



Calculating free energies

Electronic component

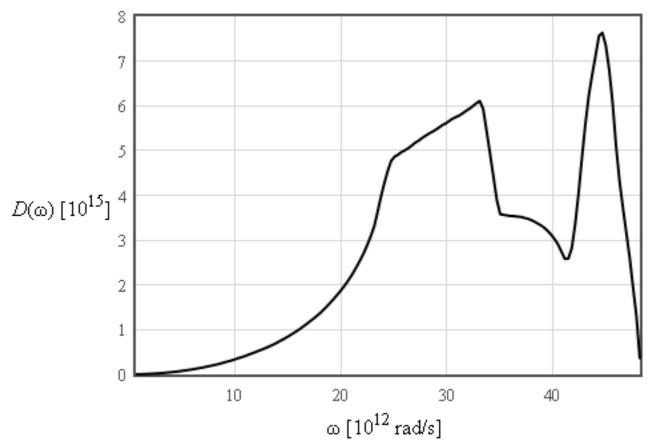


$$n = \int_{-\infty}^{\infty} \frac{D(E)}{1+\exp\left(\frac{E-\mu}{k_B T}\right)} dE$$

$$u = \int_{-\infty}^{\infty} \frac{E D(E)}{1+\exp\left(\frac{E-\mu}{k_B T}\right)} dE$$

Phonon component

$$u = \int_{-\infty}^{\infty} \frac{E D(E)}{\exp\left(\frac{E-\mu}{k_B T}\right) - 1} dE$$



Internal energy

$$U(S, N_i, M, P, \varepsilon)$$

The internal energy is a function of the extrinsic variables

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

Helmholtz free energy

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

$$F = U - TS$$

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

$$dF = \frac{\partial F}{\partial T} dT + \frac{\partial F}{\partial N_i} dN_i + \frac{\partial F}{\partial \varepsilon_{ij}} d\varepsilon_{ij} + \frac{\partial F}{\partial P_K} dP_k + \frac{\partial F}{\partial M_l} dM_l$$

$$dF = dU - TdS - SdT$$

$$dF = -SdT + \mu_i dN_i + \sigma_{ij} d\varepsilon_{ij} + E_k dP_k + H_l dM_l$$

$$S = -\left(\frac{\partial F}{\partial T}\right)_{N,M,P,\varepsilon} \qquad \mu_i = \left(\frac{\partial F}{\partial N_i}\right)_{T,M,P,\varepsilon,N_{j\neq i}} \qquad \sigma_{ij} = \left(\frac{\partial F}{\partial \varepsilon_{ij}}\right)_{N,M,P,T}$$

$$E_k = \left(\frac{\partial F}{\partial P_k}\right)_{N,M,T,\varepsilon} \qquad H_l = \left(\frac{\partial F}{\partial M_l}\right)_{N,T,P,\varepsilon}$$

Gibbs free energy

$$G(T, \mu, H, E, \sigma)$$

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

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

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

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

$$S = -\left(\frac{\partial G}{\partial T}\right)_{\sigma,E,H,\mu} \qquad N_i = -\left(\frac{\partial G}{\partial \mu_i}\right)_{T,E,H,\sigma} \qquad \varepsilon_{ij} = -\left(\frac{\partial G}{\partial \sigma_{ij}}\right)_{T,E,H,\mu}$$

$$P_k = -\left(\frac{\partial G}{\partial E_k}\right)_{T,\mu,H,\sigma} \qquad M_l = -\left(\frac{\partial G}{\partial H_l}\right)_{T,\mu,E,\sigma}$$

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

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

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

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

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3. Reciprocal (or converse) piezo-magnetic effect.
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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.
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International Tables for Crystallography
Volume D: Physical properties of crystals

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Edited by A. Authier

Contents

Groups

Crystals can have symmetries: translation, rotation, reflection, inversion,...

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & \sin\alpha \\ 0 & -\sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Symmetries can be represented by matrices.
All such matrices that bring the crystal into itself form the group of the crystal.

$$A, B \in G \qquad AB \in G$$

32 point groups (one point remains fixed during transformation)
230 space groups

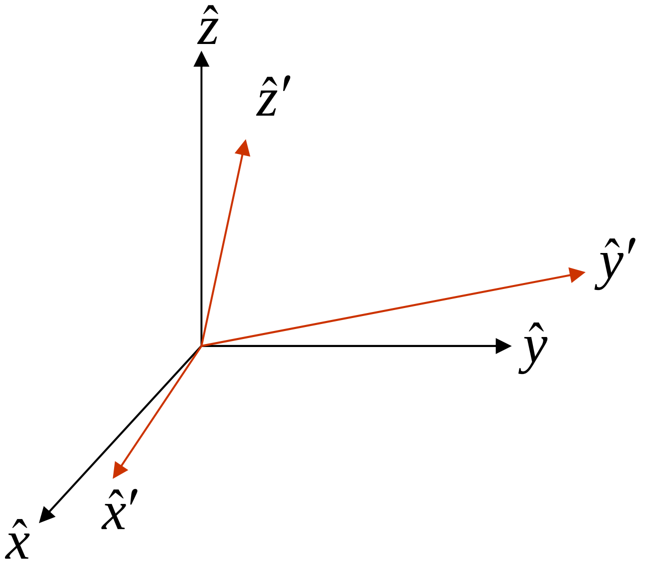
Strain

A distortion of a material is described by the strain matrix

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

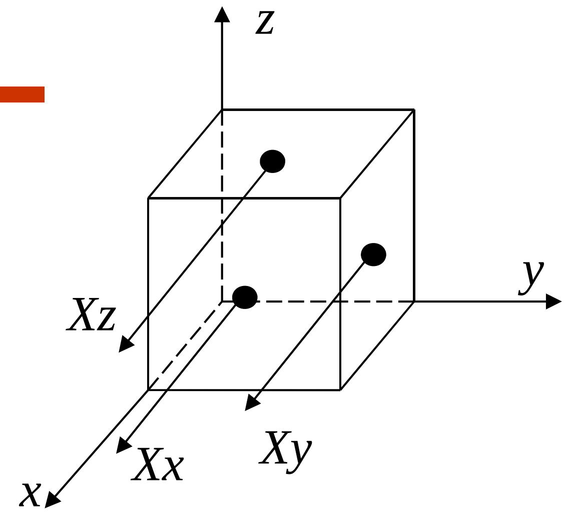
$$y' = \varepsilon_{yx}\hat{x} + (1 + \varepsilon_{yy})\hat{y} + \varepsilon_{yz}\hat{z}$$

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



Strain is dimensionless $\Delta L/L$

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.

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