

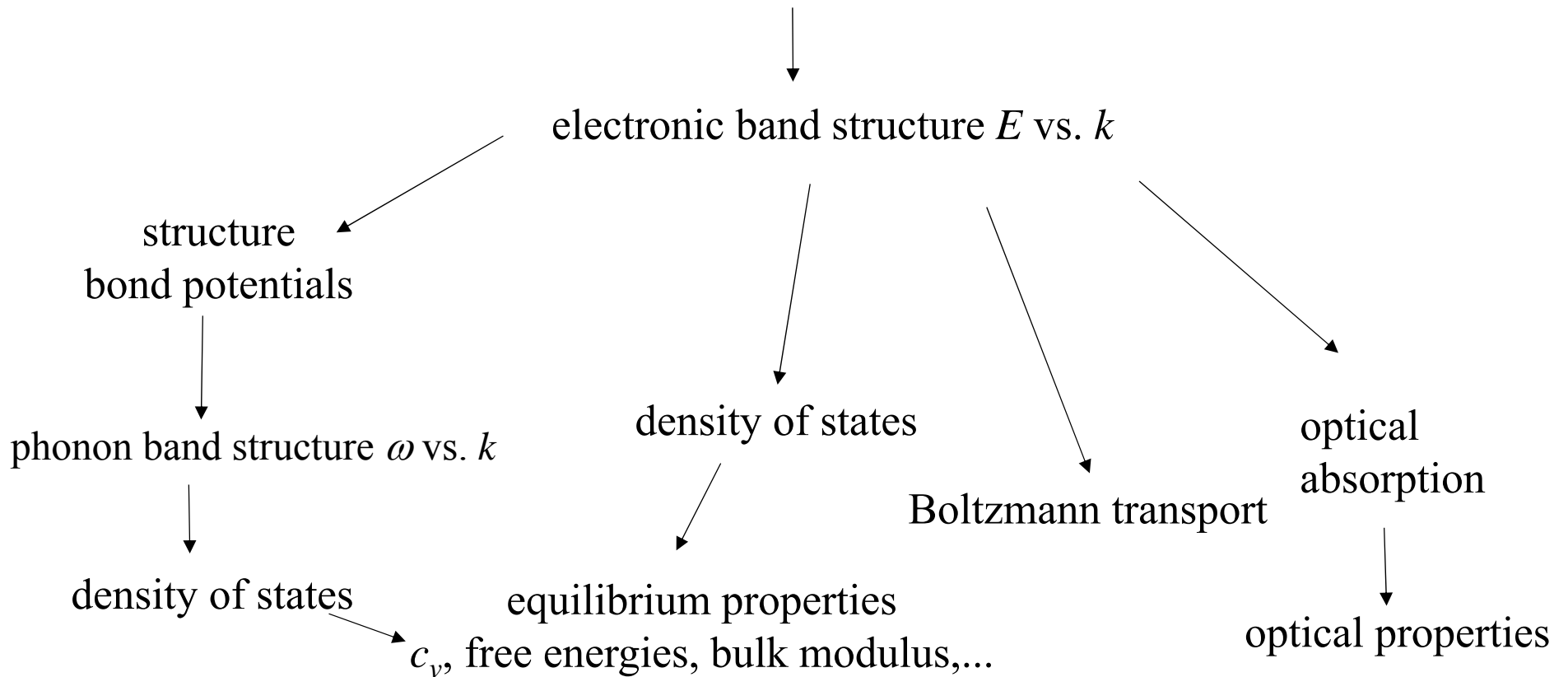
# Crystal Physics

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# The properties of solids

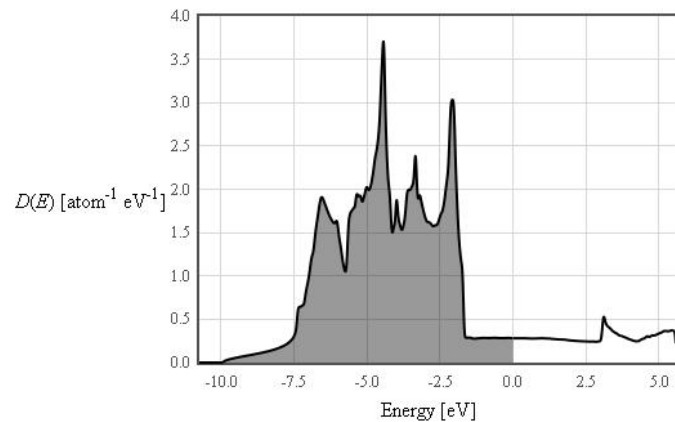
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$$H = -\sum_i \frac{\hbar^2}{2m_e} \nabla_i^2 - \sum_A \frac{\hbar^2}{2m_A} \nabla_A^2 - \sum_{i,A} \frac{Z_A e^2}{4\pi\epsilon_0 r_{iA}} + \sum_{i<j} \frac{e^2}{4\pi\epsilon_0 r_{ij}} + \sum_{A<B} \frac{Z_A Z_B e^2}{4\pi\epsilon_0 r_{AB}}$$



# Calculating free energies

## Electronic component

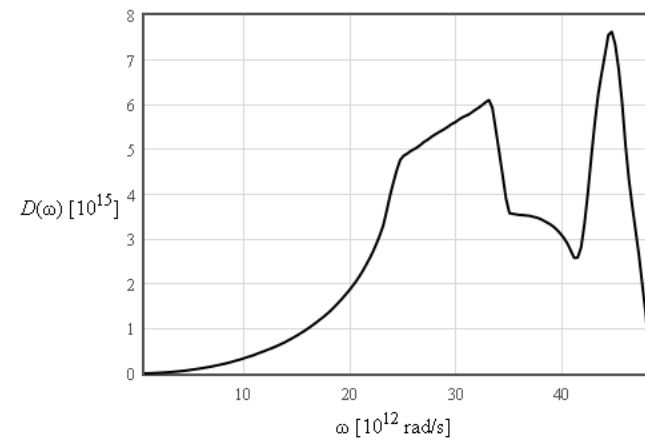


$$n = \int_{-\infty}^{\infty} \frac{D(E)}{1 + \exp\left(\frac{E - \mu}{k_B T}\right)} dE$$

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

## Phonon component

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



# Internal energy

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

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

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

$$F = U - TS$$

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

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

$$dF = dU - TdS - SdT$$

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

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

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

# Gibbs free energy

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

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

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

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

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

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

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

$$\begin{aligned}
d\epsilon_{ij} &= \left(\frac{\partial \epsilon_{ij}}{\partial \sigma_{kl}}\right) d\sigma_{kl} + \left(\frac{\partial \epsilon_{ij}}{\partial E_k}\right) dE_k + \left(\frac{\partial \epsilon_{ij}}{\partial H_l}\right) dH_l + \left(\frac{\partial \epsilon_{ij}}{\partial T}\right) dT \\
dP_i &= \left(\frac{\partial P_i}{\partial \sigma_{kl}}\right) d\sigma_{kl} + \left(\frac{\partial P_i}{\partial E_k}\right) dE_k + \left(\frac{\partial P_i}{\partial H_l}\right) dH_l + \left(\frac{\partial P_i}{\partial T}\right) dT \\
dM_i &= \left(\frac{\partial M_i}{\partial \sigma_{kl}}\right) d\sigma_{kl} + \left(\frac{\partial M_i}{\partial E_k}\right) dE_k + \left(\frac{\partial M_i}{\partial H_l}\right) dH_l + \left(\frac{\partial M_i}{\partial T}\right) dT \\
dS &= \left(\frac{\partial S}{\partial \sigma_{kl}}\right) d\sigma_{kl} + \left(\frac{\partial S}{\partial E_k}\right) dE_k + \left(\frac{\partial S}{\partial H_l}\right) dH_l + \left(\frac{\partial S}{\partial T}\right) dT
\end{aligned}$$

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.

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## International Tables for Crystallography Volume D: Physical properties of crystals

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Edited by **A. Authier**

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# Groups

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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.

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

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

# Strain

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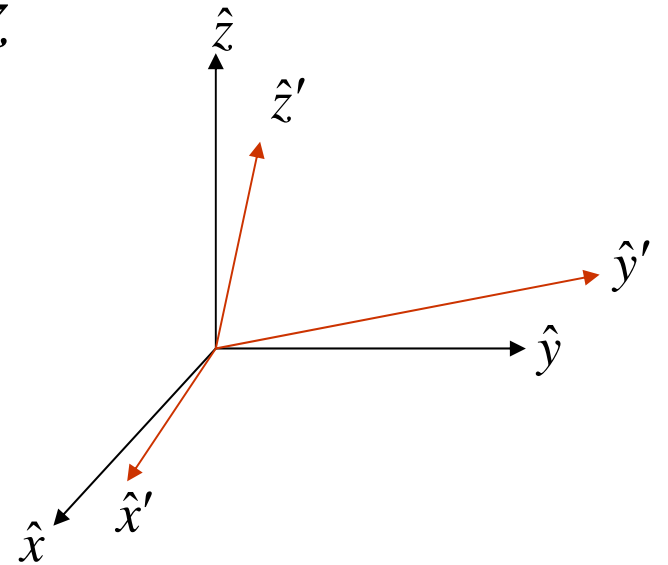
A distortion of a material is described by the strain matrix

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

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

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

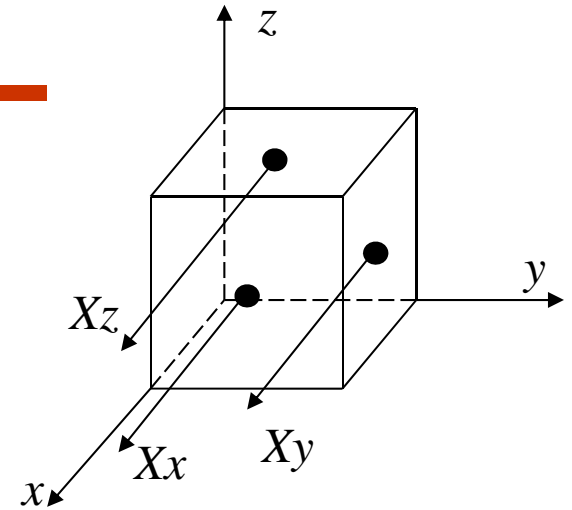
Strain is dimensionless  $\Delta L/L$



# Stress

9 forces describe the stress

$X_x, X_y, X_z, Y_x, Y_y, Y_z, Z_x, Z_y, Z_z$



$X_x$  is a force applied in the  $x$ -direction to the plane normal to  $x$

$X_y$  is a shear 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<sup>2</sup>

# Stress and Strain

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$$\epsilon_{ij} = S_{ijkl} \sigma_{kl}$$

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

$$\sigma_{ij} = C_{ijkl} \epsilon_{kl}$$

Einstein convention: sum over repeated indices.

$$\begin{aligned} \epsilon_{xx} = & S_{xxxx} \sigma_{xx} + S_{xxxy} \sigma_{xy} + S_{xxxz} \sigma_{xz} + S_{xxyx} \sigma_{yx} + S_{xxyy} \sigma_{yy} \\ & + S_{xxyz} \sigma_{yz} + S_{xxzx} \sigma_{zx} + S_{xxzy} \sigma_{zy} + S_{xxzz} \sigma_{zz} \end{aligned}$$