

Crystal Physics

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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

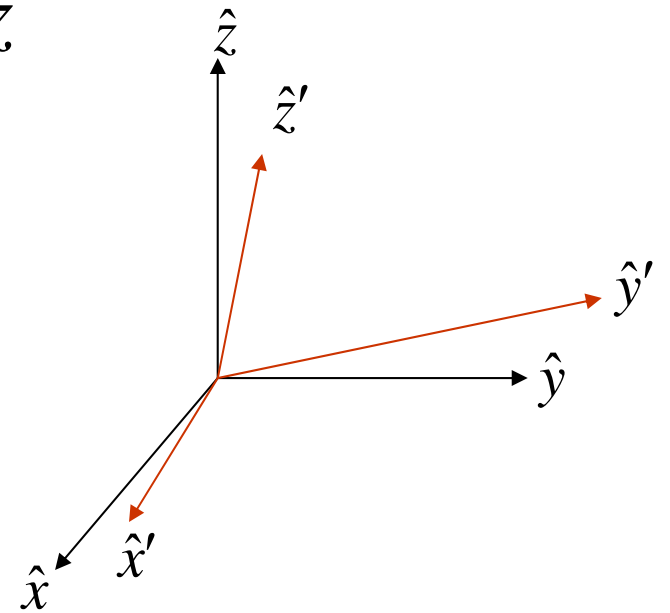
Strain

A distortion of a material is described by the strain matrix

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

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

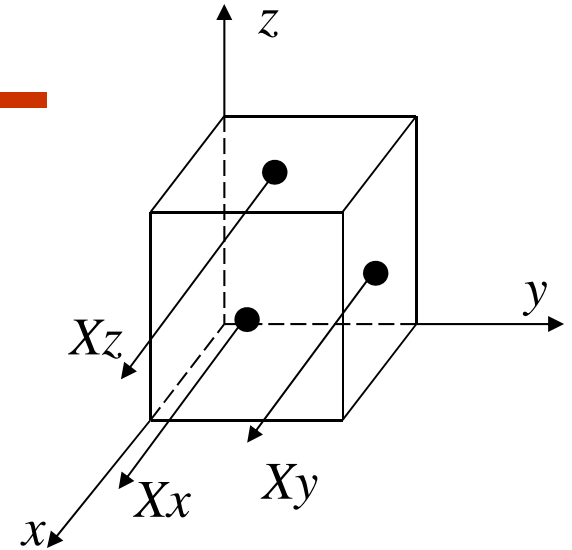
$$z' = \varepsilon_{zx}\hat{x} + \varepsilon_{zy}\hat{y} + (1 + \varepsilon_{zz})\hat{z}$$



Stress

9 forces describe the stress

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



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/m²

Stress and Strain

$$\boldsymbol{\varepsilon}_{ij} = S_{ijkl} \boldsymbol{\sigma}_{kl}$$

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

$$\boldsymbol{\sigma}_{ij} = C_{ijkl} \boldsymbol{\varepsilon}_{kl}$$

Einstein convention: sum over repeated indices.

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

Statistical Physics

Microcanonical 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.

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

$$E_k = \frac{\partial U}{\partial P_k}$$

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

Statistical Physics

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

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

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

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

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

Helmholtz free energy

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

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

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

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

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

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

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

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

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

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.

Direct and reciprocal effects (Maxwell relations)

$$-\left(\frac{\partial^2 G}{\partial \sigma_{ij} \partial E_k}\right) = \left(\frac{\partial P_k}{\partial \sigma_{ij}}\right) = -\left(\frac{\partial^2 G}{\partial E_k \partial \sigma_{ij}}\right) = \left(\frac{\partial \epsilon_{ij}}{\partial E_k}\right) = d_{kij}$$

$$-\left(\frac{\partial^2 G}{\partial \sigma_{ij} \partial H_l}\right) = \left(\frac{\partial M_l}{\partial \sigma_{ij}}\right) = -\left(\frac{\partial^2 G}{\partial H_l \partial \sigma_{ij}}\right) = \left(\frac{\partial \epsilon_{ij}}{\partial H_l}\right) = g_{lij}$$

$$-\left(\frac{\partial^2 G}{\partial E_k \partial H_l}\right) = \left(\frac{\partial M_l}{\partial E_k}\right) = -\left(\frac{\partial^2 G}{\partial H_l \partial E_k}\right) = \left(\frac{\partial P_k}{\partial H_l}\right) = \lambda_{lk}$$

$$-\left(\frac{\partial^2 G}{\partial \sigma_{ij} \partial T}\right) = \left(\frac{\partial S}{\partial \sigma_{ij}}\right) = -\left(\frac{\partial^2 G}{\partial T \partial \sigma_{ij}}\right) = \left(\frac{\partial \epsilon_{ij}}{\partial T}\right) = \alpha_{ij}$$

$$-\left(\frac{\partial^2 G}{\partial T \partial E_k}\right) = \left(\frac{\partial P_k}{\partial T}\right) = -\left(\frac{\partial^2 G}{\partial E_k \partial T}\right) = \left(\frac{\partial S}{\partial E_k}\right) = p_k$$

$$-\left(\frac{\partial^2 G}{\partial T \partial H_l}\right) = \left(\frac{\partial M_l}{\partial T}\right) = -\left(\frac{\partial^2 G}{\partial H_l \partial T}\right) = \left(\frac{\partial S}{\partial H_l}\right) = m_l.$$

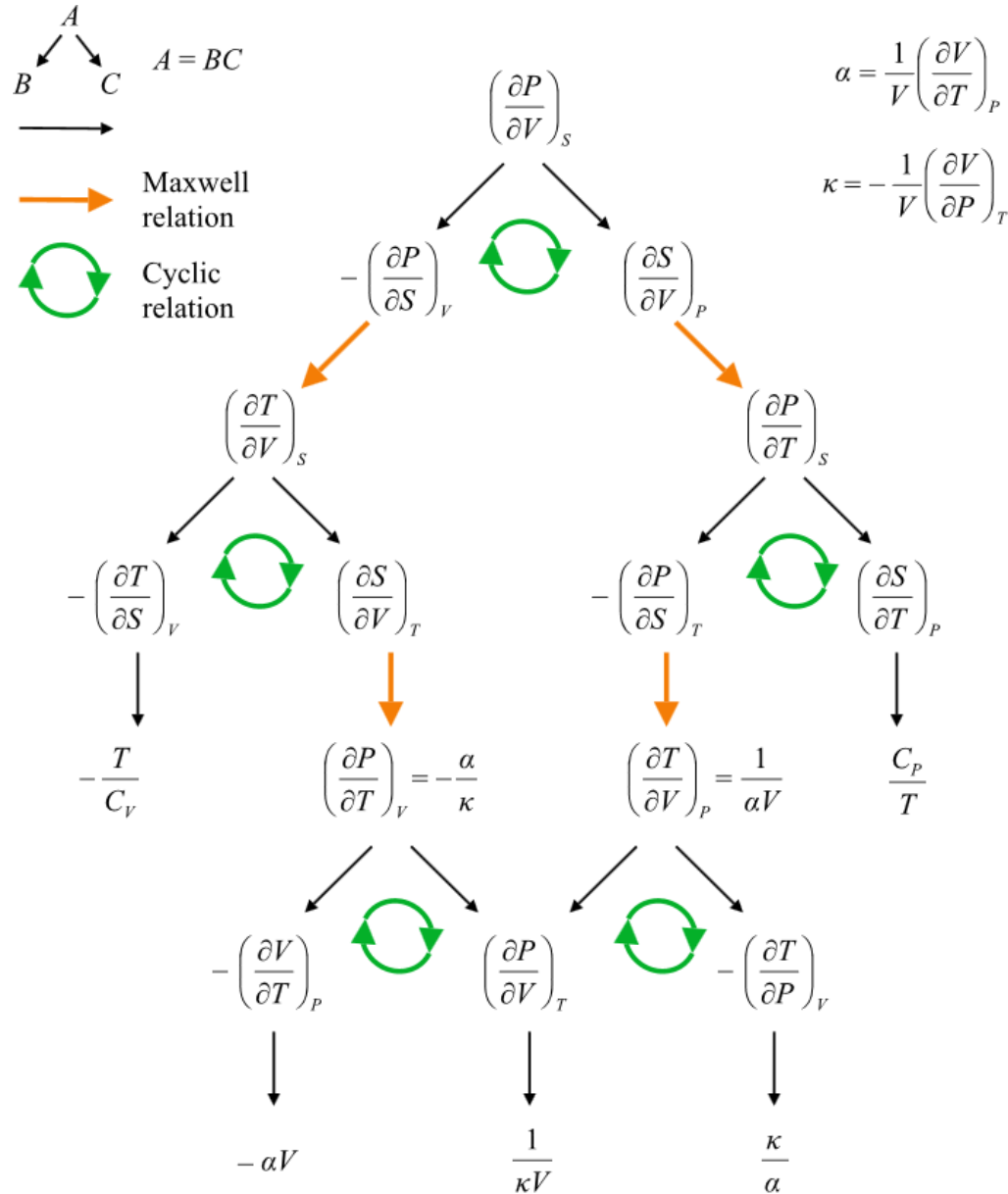
Useful to check for errors in experiments or calculations

Maxwell relations

$$\begin{aligned} + \left(\frac{\partial T}{\partial V} \right)_S &= - \left(\frac{\partial P}{\partial S} \right)_V = \frac{\partial^2 U}{\partial S \partial V} \\ + \left(\frac{\partial T}{\partial P} \right)_S &= + \left(\frac{\partial V}{\partial S} \right)_P = \frac{\partial^2 H}{\partial S \partial P} \\ + \left(\frac{\partial S}{\partial V} \right)_T &= + \left(\frac{\partial P}{\partial T} \right)_V = - \frac{\partial^2 F}{\partial T \partial V} \\ - \left(\frac{\partial S}{\partial P} \right)_T &= + \left(\frac{\partial V}{\partial T} \right)_P = \frac{\partial^2 G}{\partial T \partial P} \end{aligned}$$

Useful to check for errors in experiments or calculations

Replace P and V with σ and ε



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Edited by **A. Authier**

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The properties of solids

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

