Symmetries, Crystal physics

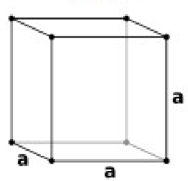
Cubic crystals

All second rank tensors of cubic crystals reduce to constants

Electrical conductivity, thermal conductivity, electric susceptibility, magnetic susceptibility, Peltier effect (heat current due to electrical current), Seebeck effect (Electric field due to thermal gradient)

216: ZnS, GaAs, GaP, InAs, SiC
221: CsCl, cubic perovskite
225: Al, Cu, Ni, Ag, Pt, Au, Pb, NaCl
227: C, Si, Ge, spinel
229: Na, K, Cr, Fe, Nb, Mo, Ta

Cubic



23	T	195-199		12
$m3$	T_h	200-206		24
432	O	207-214		24
$\bar{4}3m$	T_d	215-220	216: Zincblende, ZnS, GaAs, GaP, InAs, SiC	24
$m3m$	O_h	221-230	221: CsCl, cubic perovskite 225: fcc, Al, Cu, Ni, Ag, Pt, Au, Pb, γ-Fe, NaCl 227: diamond, C, Si,	48

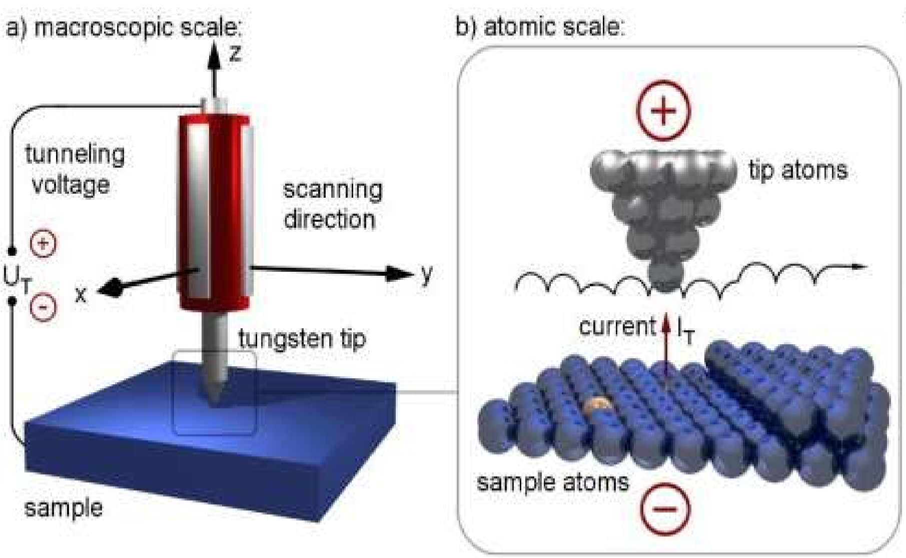
$$\begin{bmatrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{11} \end{bmatrix}$$

Piezoelectricity (rank 3 tensor)

AFM's, STM's
Quartz crystal oscillators
Surface acoustic wave generators
Pressure sensors - Epcos
Fuel injectors - Bosch
Inkjet printers

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

No inversion symmetry



lead zirconate titanate ($Pb[Zr_xTi_{1-x}]O_3$ $0<x<1$)
—more commonly known as PZT
barium titanate ($BaTiO_3$)
lead titanate ($PbTiO_3$)
potassium niobate ($KNbO_3$)
lithium niobate ($LiNbO_3$)
lithium tantalate ($LiTaO_3$)
sodium tungstate (Na_2WO_3)
$Ba_2NaNb_5O_5$
$Pb_2KNb_5O_{15}$

Piezoelectric crystal classes: 1, 2, m, 222, mm2, 4, -4, 422, 4mm, -42m, 3, 32, 3m, 6, -6, 622, 6mm, -62m, 23, -43m

Electrostriction

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

$$\boldsymbol{\epsilon_{ij} = d_{ijk} E_k + Q_{ijkl} E_k E_l + \cdots}$$

piezoelectricity

Electrostriction

Nonlinear optics

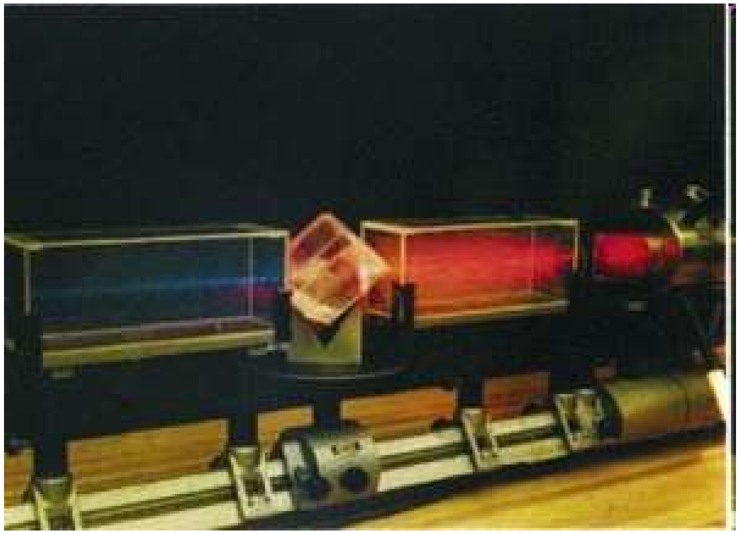
Period doubling crystals

no inversion symmetry

$$P = \chi^{(1)}E + \chi^{(2)}E^2 + \chi^{(3)}E^3 + \cdots$$

$$P_i = \frac{-\partial^2 G}{\partial E_i \partial E_j} E_j + \frac{1}{2} \frac{-\partial^3 G}{\partial E_i \partial E_j \partial E_k} E_j E_k + \cdots$$

$$\cos^2(\omega t) = \tfrac{1}{2}\left(1 + \cos(2\omega t)\right)$$



806 nm light : lithium iodate ($LiIO_3$)
860 nm light : potassium niobate ($KNbO_3$)
980 nm light : $KNbO_3$
1064 nm light : monopotassium phosphate (KH_2PO_4, KDP), lithium triborate (LBO).
1300 nm light : gallium selenide (GaSe)
1319 nm light : $KNbO_3$, BBO, KDP, lithium niobate ($LiNbO_3$), $LiIO_3$

Symmetric Tensors

$$\chi_{ij}^{E} = \frac{\partial P_i}{\partial E_j} = -\frac{\partial^2 G}{\partial E_i \partial E_j} = \frac{\partial P_j}{\partial E_i} = \chi_{ji}^{E}$$

$$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{12} & g_{22} & g_{23} \\ g_{13} & g_{23} & g_{33} \end{bmatrix}$$

Tensor notation

We need a way to represent 3rd and 4th rank tensors in 2-d.

$$1\,1 \rightarrow 1 \quad 1\,2 \rightarrow 6 \quad 1\,3 \rightarrow 5$$

$$2\,2 \rightarrow 2 \quad 2\,3 \rightarrow 4$$

$$3\,3 \rightarrow 3$$

rank 3

$$g_{36} \rightarrow g_{312}$$

rank 4

$$g_{14} \rightarrow g_{1123}$$

rank 2 symmetric tensors[2]	rank 2 asymmetric tensors	rank 3 tensors[3]	rank 4 tensors
$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{12} & g_{22} & g_{23} \\ g_{13} & g_{23} & g_{33} \end{bmatrix}$	$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{bmatrix}$	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & g_{14} & g_{15} & g_{16} \\ g_{21} & g_{22} & g_{23} & g_{24} & g_{25} & g_{26} \\ g_{31} & g_{32} & g_{33} & g_{34} & g_{35} & g_{36} \end{bmatrix}$ reduced, symmetric, asymmetric	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & g_{14} & g_{15} & g_{16} \\ g_{21} & g_{22} & g_{23} & g_{24} & g_{25} & g_{26} \\ g_{31} & g_{32} & g_{33} & g_{34} & g_{35} & g_{36} \\ g_{41} & g_{42} & g_{43} & g_{44} & g_{45} & g_{46} \\ g_{51} & g_{52} & g_{53} & g_{54} & g_{55} & g_{56} \\ g_{61} & g_{62} & g_{63} & g_{64} & g_{65} & g_{66} \end{bmatrix}$ reduced, symmetric, asymmetric
	$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ reduced, symmetric, asymmetric	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & g_{14} & g_{15} & g_{16} \\ g_{21} & g_{22} & g_{23} & g_{24} & g_{25} & g_{26} \\ g_{31} & g_{32} & g_{33} & g_{34} & g_{35} & g_{36} \\ g_{41} & g_{42} & g_{43} & g_{44} & g_{45} & g_{46} \\ g_{51} & g_{52} & g_{53} & g_{54} & g_{55} & g_{56} \\ g_{61} & g_{62} & g_{63} & g_{64} & g_{65} & g_{66} \end{bmatrix}$ reduced, symmetric, asymmetric
$\begin{bmatrix} g_{11} & g_{12} & 0 \\ g_{12} & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} g_{11} & g_{12} & 0 \\ g_{21} & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 & g_{14} & g_{15} & 0 \\ 0 & 0 & 0 & g_{24} & g_{25} & 0 \\ g_{31} & g_{32} & g_{33} & 0 & 0 & g_{36} \end{bmatrix}$ reduced, symmetric, asymmetric	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & 0 & 0 & g_{16} \\ g_{21} & g_{22} & g_{23} & 0 & 0 & g_{26} \\ g_{31} & g_{32} & g_{33} & 0 & 0 & g_{36} \\ 0 & 0 & 0 & g_{44} & g_{45} & 0 \\ 0 & 0 & 0 & g_{54} & g_{55} & 0 \\ g_{61} & g_{62} & g_{63} & 0 & 0 & g_{66} \end{bmatrix}$ reduced, symmetric, asymmetric
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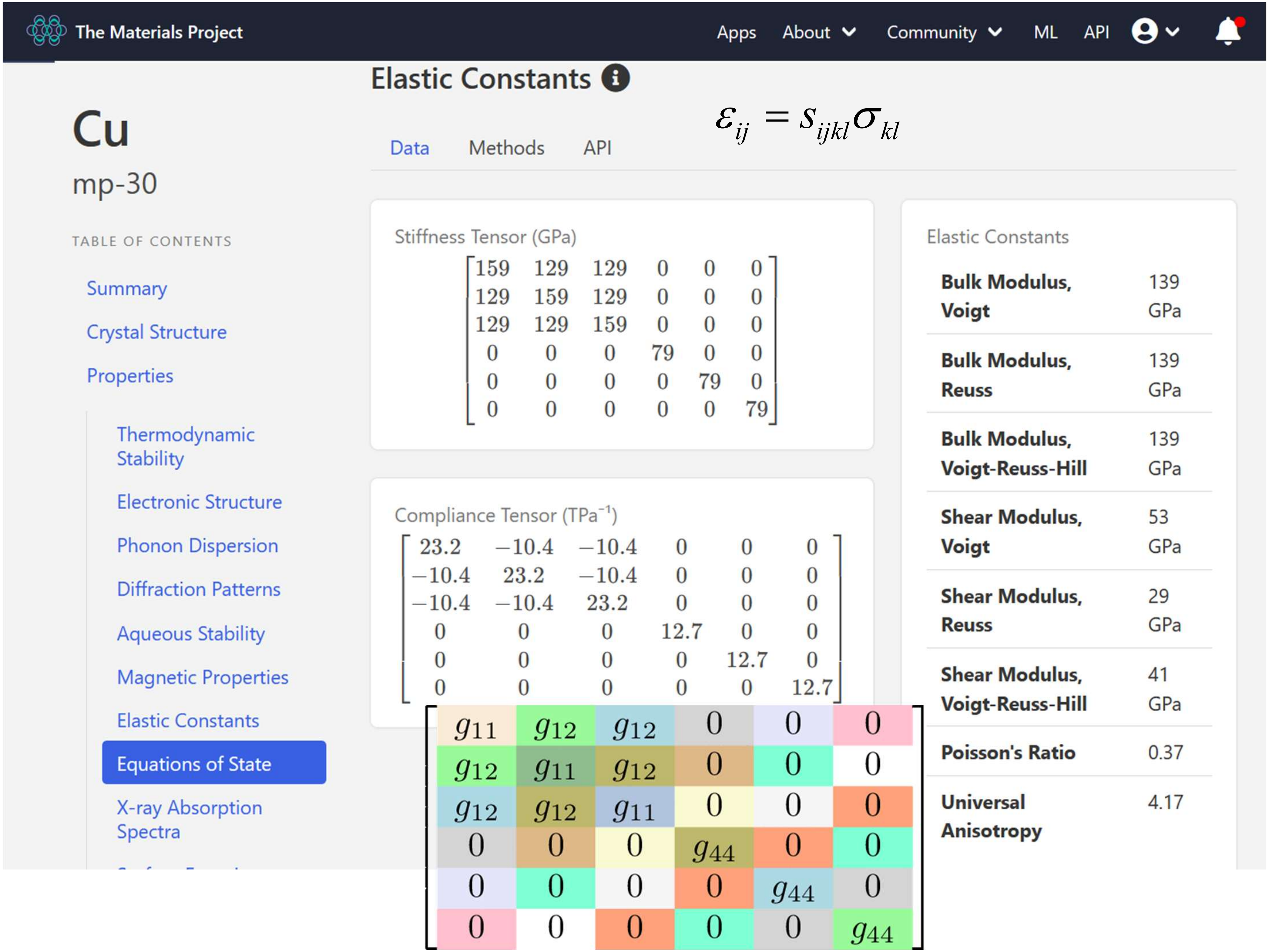
	$\begin{bmatrix} g_{11} & g_{12} & 0 \\ g_{21} & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ reduced, symmetric, asymmetric	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & 0 & 0 & g_{16} \\ g_{21} & g_{22} & g_{23} & 0 & 0 & g_{26} \\ g_{31} & g_{32} & g_{33} & 0 & 0 & g_{36} \\ 0 & 0 & 0 & g_{44} & g_{45} & 0 \\ 0 & 0 & 0 & g_{54} & g_{55} & 0 \\ g_{61} & g_{62} & g_{63} & 0 & 0 & g_{66} \end{bmatrix}$ reduced, symmetric, asymmetric
rank 2 symmetric tensors[2]	rank 2 asymmetric tensors	rank 3 tensors[3]	rank 4 tensors
	$\begin{bmatrix} g_{11} & 0 & 0 \\ 0 & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 & g_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & g_{25} & 0 \\ 0 & 0 & 0 & 0 & 0 & g_{36} \end{bmatrix}$ reduced, symmetric, asymmetric	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & 0 & 0 & 0 \\ g_{21} & g_{22} & g_{23} & 0 & 0 & 0 \\ g_{31} & g_{32} & g_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & g_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & g_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & g_{66} \end{bmatrix}$ reduced, symmetric, asymmetric

http://lamp.tu-graz.ac.at/~hadley/ss2/crystalphysics/crystalclasses/crystalclasses.html



The Materials Project
Apps
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Community
ML
API
Elastic Constants
$\varepsilon_{ij} = s_{ijkl}\sigma_{kl}$
Cu
mp-30
Data
Methods
API
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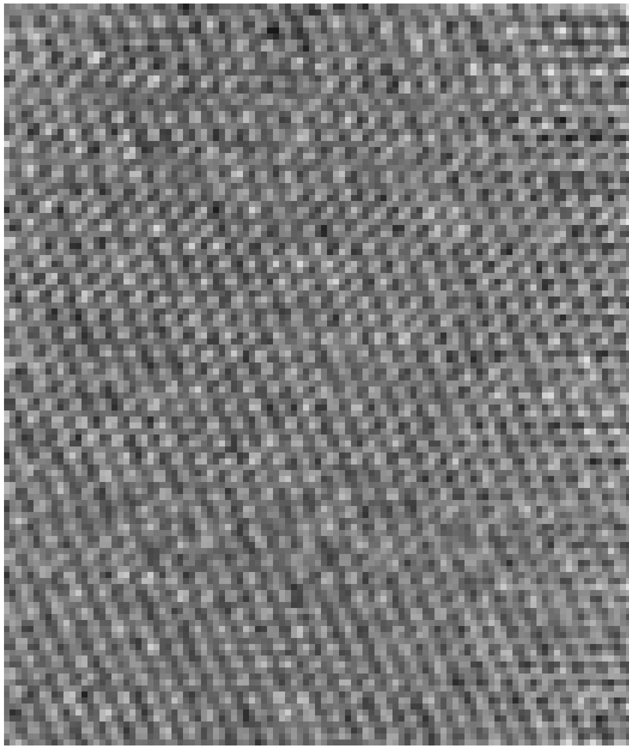
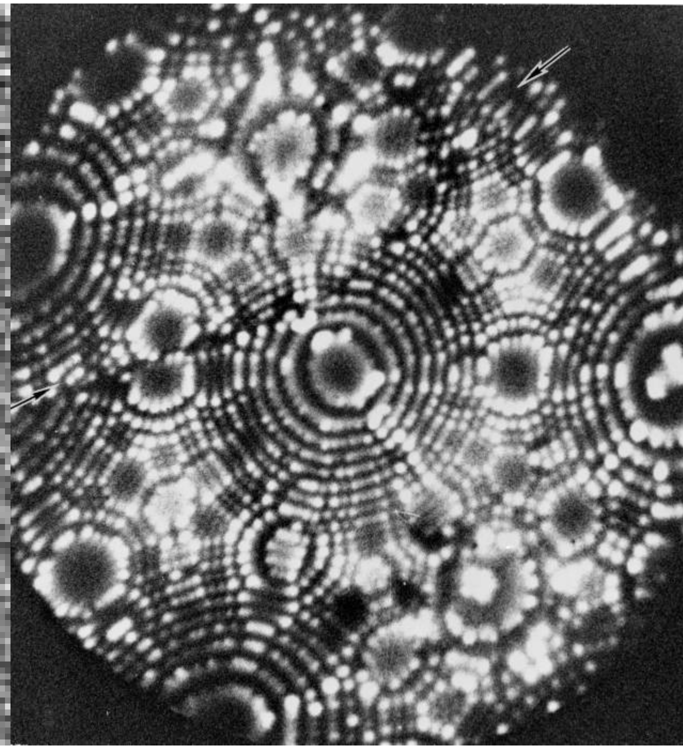
Equations of State
X-ray Absorption Spectra
Stiffness Tensor (GPa)
$\begin{bmatrix} 159 & 129 & 129 & 0 & 0 & 0 \\ 129 & 159 & 129 & 0 & 0 & 0 \\ 129 & 129 & 159 & 0 & 0 & 0 \\ 0 & 0 & 0 & 79 & 0 & 0 \\ 0 & 0 & 0 & 0 & 79 & 0 \\ 0 & 0 & 0 & 0 & 0 & 79 \end{bmatrix}$
Compliance Tensor (TPa^{-1})
$\begin{bmatrix} 23.2 & -10.4 & -10.4 & 0 & 0 & 0 \\ -10.4 & 23.2 & -10.4 & 0 & 0 & 0 \\ -10.4 & -10.4 & 23.2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 12.7 & 0 & 0 \\ 0 & 0 & 0 & 0 & 12.7 & 0 \\ 0 & 0 & 0 & 0 & 0 & 12.7 \end{bmatrix}$
$\begin{bmatrix} g_{11} & g_{12} & g_{12} & 0 & 0 & 0 \\ g_{12} & g_{11} & g_{12} & 0 & 0 & 0 \\ g_{12} & g_{12} & g_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & g_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & g_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & g_{44} \end{bmatrix}$
Elastic Constants
Bulk Modulus, Voigt 139 GPa
Bulk Modulus, Reuss 139 GPa
Bulk Modulus, Voigt-Reuss-Hill 139 GPa
Shear Modulus, Voigt 53 GPa
Shear Modulus, Reuss 29 GPa
Shear Modulus, Voigt-Reuss-Hill 41 GPa
Poisson's Ratio 0.37
Universal Anisotropy 4.17

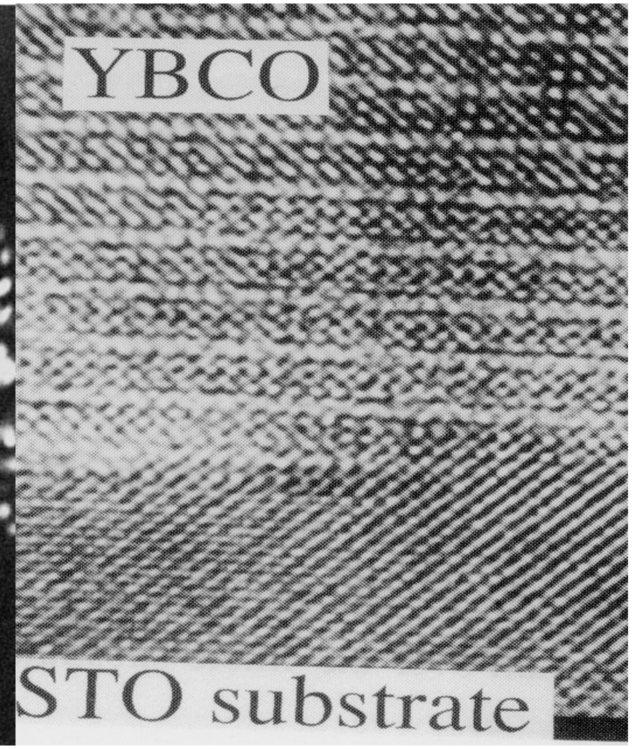
Crystal structure determination



Scanning tunneling microscope



Field ion microscope



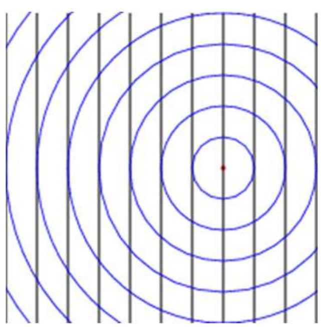
Transmission electron microscope

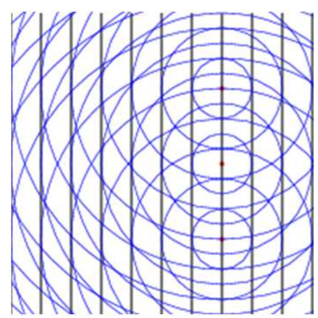
Usually x-ray diffraction is used to determine the crystal structure

Crystal diffraction (Beugung)

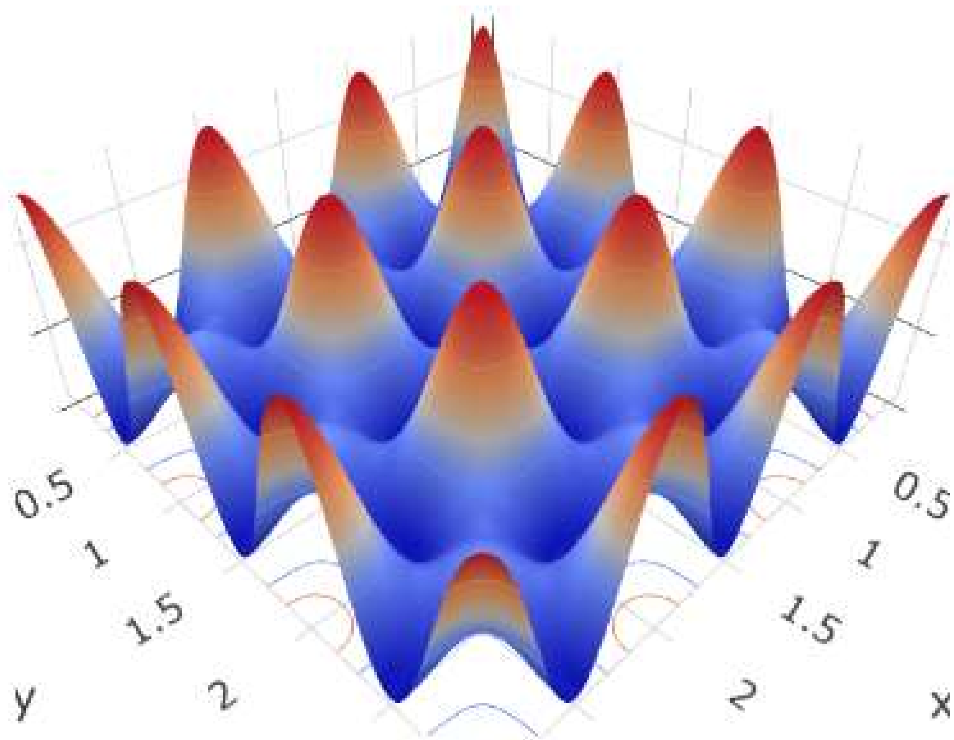
Everything moves like a wave but exchanges energy and momentum as a particle

light	photons
sound	phonons
electron waves	electrons
neutron waves	neutrons
positron waves	positrons
plasma waves	plasmons



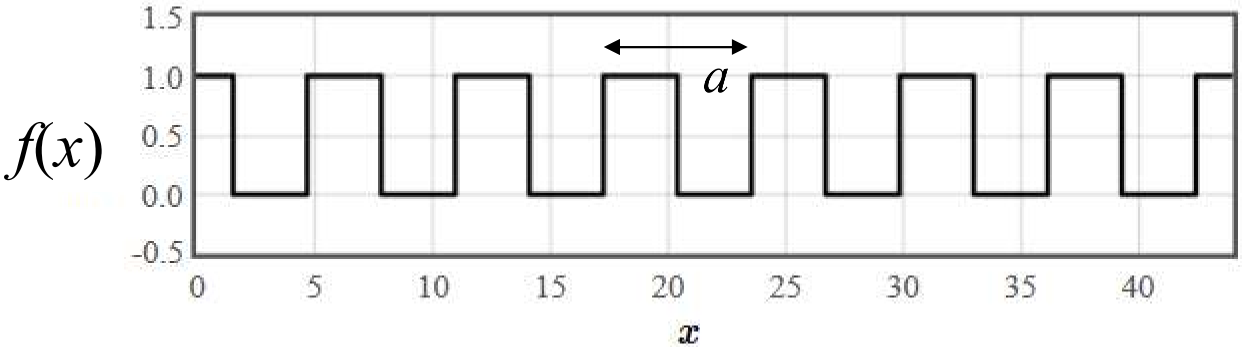


Periodic functions



Use a Fourier series to describe periodic functions

Expanding a 1-d function in a Fourier series



Any periodic function can be represented as a Fourier series.

$$f(x) = f_0 + \sum_{p=1}^{\infty} c_p \cos(2\pi px/a) + s_p \sin(2\pi px/a)$$

multiply by $\cos(2\pi p'x/a)$ and integrate over a period.

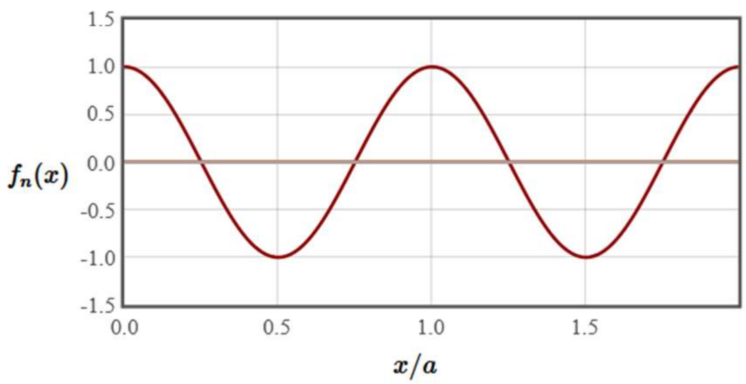
$$\int_0^a f(x)\cos\left(2\pi p'x/a\right)dx = c_p \int_0^a \cos\left(2\pi p'x/a\right)\cos\left(2\pi p'x/a\right)dx = \frac{ac_{p'}}{2}$$

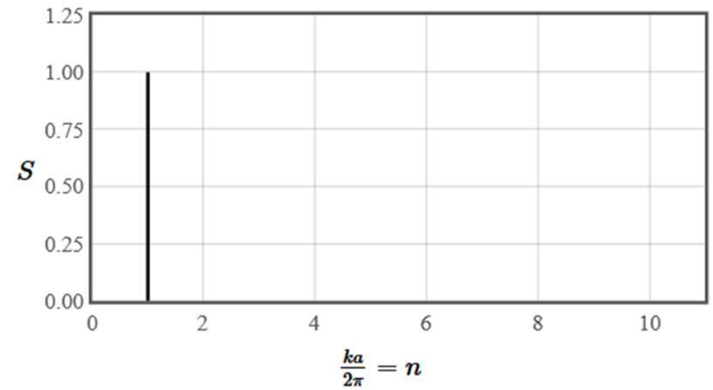
$$c_p = \frac{2}{a}\int_0^a f(x)\cos\left(2\pi px/a\right)dx$$

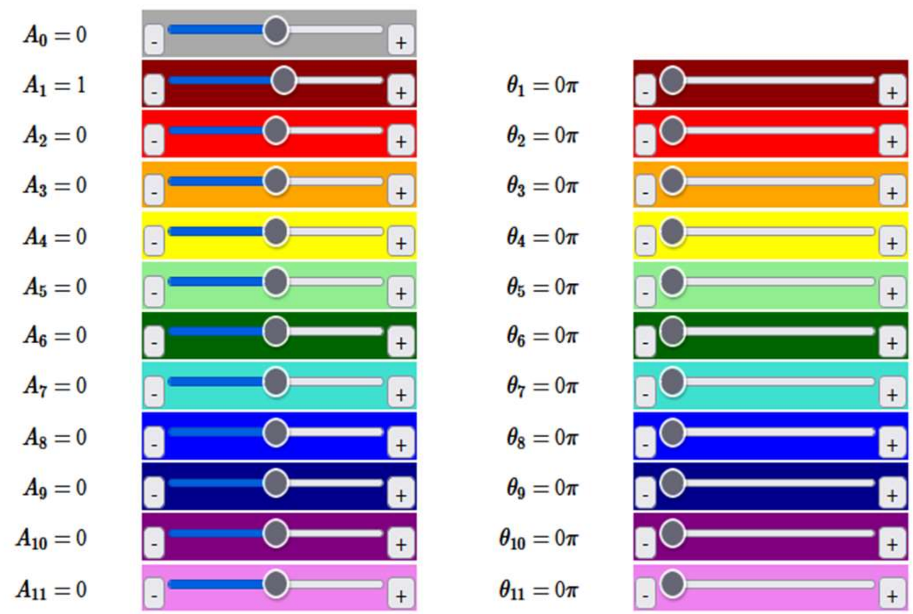
Fourier synthesis

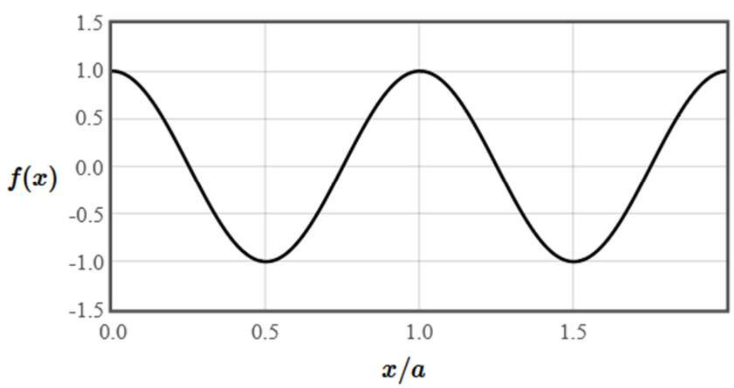
A periodic function with period a can be written as a Fourier series of the form,

$$f(x) = A_0 + \sum_n A_n \left(\cos(\theta_n)\cos(2\pi n x/a) + \sin(\theta_n)\sin(2\pi n x/a)\right).$$



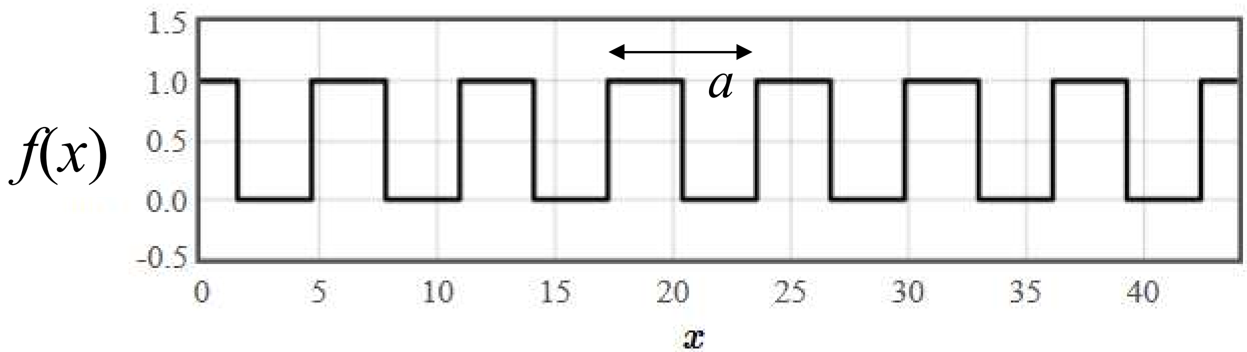






Number of periods displayed: 2

Expanding a 1-d function in a Fourier series



Any periodic function can be represented as a Fourier series.

$$f(x) = f_0 + \sum_{p=1}^{\infty} c_p \cos(2\pi px/a) + s_p \sin(2\pi px/a)$$

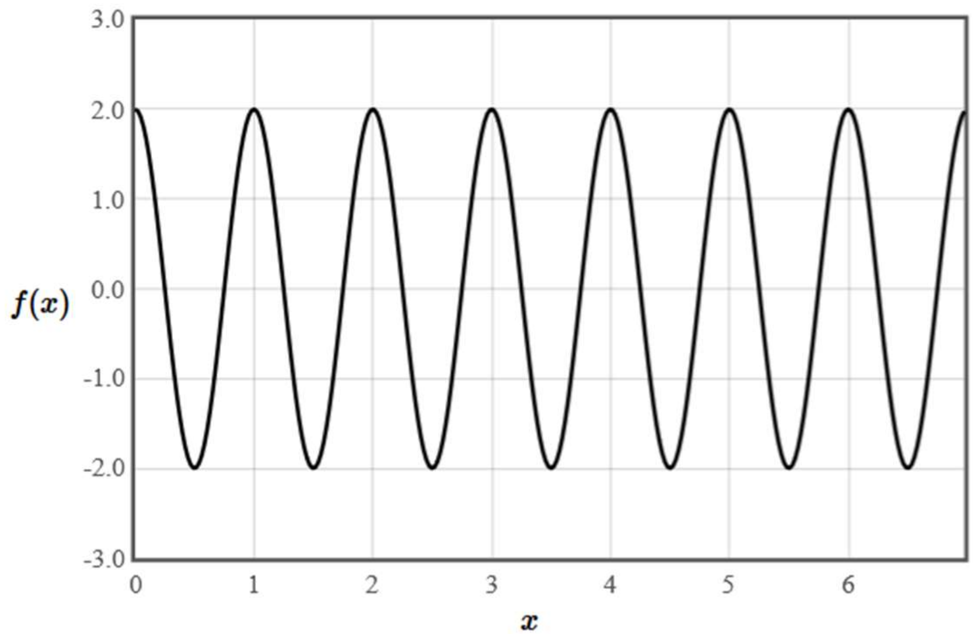
$$\cos x = \frac{e^{ix} + e^{-ix}}{2} \qquad \sin x = \frac{e^{ix} - e^{-ix}}{2i}$$

$$f(x) = \sum_{G=-\infty}^{\infty} f_G e^{iGx} \qquad f_G = \frac{c_p}{2} - i\frac{s_p}{2} \qquad G = \frac{2\pi p}{a}$$

For real functions: $f_G^* = f_{-G}$

reciprocal lattice vector

Fourier series in 1-D



square triangle sawtooth comb

$f_0 = 0$ - +

$f_1 = f^*_{-1} = 1$ - + $+i\ (0)$ - +

$f_2 = f^*_{-2} = 0$ - + $+i\ (0)$ - +

$f_3 = f^*_{-3} = 0$ - + $+i\ (0)$ - +

$f_4 = f^*_{-4} = 0$ - + $+i\ (0)$ - +

$f_5 = f^*_{-5} = 0$ - + $+i\ (0)$ - +

Determine the Fourier coefficients in 1-D

$$f(x) = \sum_{G} f_G e^{iGx}$$

Multiply by $e^{-iG'x}$ and integrate over a period a

$$\int_{\text{unit cell}} f(x)\, e^{-iG'}\ dx = \int_{unit\ cell} \sum_{G} f_G e^{i(G-G')x} dx \quad = f_{G'} a$$

$$f_G = \frac{1}{a} \int_{-\infty}^{\infty} f_{cell}(x) e^{-iGx} dx$$

The Fourier coefficient is proportional to the Fourier transform of the pattern that gets repeated on the Bravais lattice, evaluated at that G-vector.

Fourier series in 1-D, 2-D, or 3-D

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

Reciprocal lattice vectors *G*
(depend on the Bravais lattice)

Structure factors
(complex numbers)

$$\vec{T}_{hkl} = h\vec{a}_1 + k\vec{a}_2 + l\vec{a}_3$$

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij} \qquad \delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0, & \text{for } i \neq j \end{cases}$$

$$\vec{G} = \nu_1\vec{b}_1 + \nu_2\vec{b}_2 + \nu_3\vec{b}_3$$