perovskite = CaTiO$_3$ (a mineral). It lends its name to the “perovskite crystal structure” (a common ABX$_3$ structure)

Each Ca atom is translationally equivalent to every other Ca atom. The same is true for Ti atoms.

These two oxygens are NOT translationally equivalent (but they are rotationally equivalent)

The site-symmetry of Ti is cubic, as is the site-symmetry of Ca. But oxygens have lower site symmetry (tetragonal.)

some “perovskites”
1. BaTiO$_3$ (ferroelectric)
2. CaMnO$_3$ (simple antiferromagnet)
3. SrRuO$_3$ (metallic ferromagnet)
4. LaMnO$_3$ (“colossal magnetoresistance)
5. (Mg$_{0.9}$Fe$_{0.1}$SiO$_3$) (dominant lower mantle mineral)

related structures:
1. La$_2$CuO$_4$ (parent of high T$_c$ cuprates)
2. Sr$_2$RuO$_4$ (“p-wave” superconductor)
Ne, Ar, K, Xe, Al, Pb, Cu, Ag, Au all crystallize in the “fcc structure.”

diamond, zincblende, and rocksalt structures all have the “fcc lattice.”

Note that the words “fcc structure” and “fcc lattice” do not mean the same thing.

Quiz: what solid has the highest melting temperature?
Crystal structure = Lattice + Basis

cesium chloride crystal structure
= simple cubic (sc) lattice
+ 2 atom basis (cesium at (0,0,0),
  chlorine at ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$))

bcc (body-centered cubic) crystal
structure = bcc lattice + 1 atom basis

V$_3$Si crystal structure ("A15 structure")
= bcc lattice + 4 atom basis (primitive
description)
= sc lattice + 8 atom basis (non-primitive
description)

$\begin{pmatrix} \vec{a}_1, \vec{a}_2, \vec{a}_3 \end{pmatrix}$ = primitive translation
vectors (not unique)!

$\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$ = volume of unit cell (unique)
but shape of unit cell is not unique
lattice sites
Wigner-Seitz cell
Bravais lattice
Fourier series (1d)

\[ f(x + l) = f(x) \]

\[ f(x) = \sum_q A_q e^{i\phi_q} \]

\[ g_n = n \frac{2\pi}{a} \]

\[ e^{i\phi_l} = 1 \]

\[ A_q = \frac{1}{a} \int_{\text{cell}} f(x) e^{-i\phi_q} \, dx \]

\[ gl = n \frac{2\pi}{a} l_1 a = nl_1 2\pi = \text{integer} \times 2\pi \]

Fourier series (3d)

\[ f(r + l) = f(r + l_x a_x + l_y a_y + l_z a_z) = f(r) \]

\[ f(r) = \sum_q A_q e^{i\phi_q} \]
Ziman's notation

**My notation:**

**primitive vectors of the reciprocal lattice**

The vectors of the reciprocal lattice:

\[ \vec{G} = n_1 \vec{G}_1 + n_2 \vec{G}_2 + n_3 \vec{G}_3 \]

The vectors of the direct lattice:

\[ \vec{\ell} = \ell_1 \vec{a}_1 + \ell_2 \vec{a}_2 + \ell_3 \vec{a}_3 \]

\[ e^{i\vec{G} \cdot \vec{\ell}} = 1 \]
Properties of the reciprocal lattice

(i) Each vector of the reciprocal lattice is normal to a set of lattice planes of the direct lattice.

(ii) If the components of \( g \) have no common factor, then \( |g| \) is inversely proportional to the spacing of the lattice planes normal to \( g \).

(iii) The volume of a unit cell of the reciprocal lattice is inversely proportional to the volume of a unit cell of the direct lattice.

\[ \Omega_G = (2\pi)^3 / \Omega_\ell \]

(iv) The direct lattice is the reciprocal of its own reciprocal lattice.

\[ \times \text{ (v) The unit cell of the reciprocal lattice need not be a parallelepiped.} \]

In fact, we almost always deal with the Wigner–Seitz cell of the reciprocal lattice. This is called a Brillouin zone.

\[ \xmark \]

my definition:

The Brillouin zone is the unit cell of reciprocal space. It's shape can be varied, subject to the constraint that the BZ must contain one and only one copy of each wavevector \( Q \), and never also a vector \( Q+G \) for nonzero \( G \).
Bloch’s Theorem

When choosing a complete set of eigenfunctions of a translationally-invariant linear equation like the Schrödinger equation, it is possible to choose them all to be simultaneous eigenfunctions of the translations, such that translation by a lattice vector \( \mathbf{l} \) is equivalent to multiplying by a phase factor: \( \psi(\mathbf{r} + \mathbf{l}) = e^{i\mathbf{k} \cdot \mathbf{l}} \psi(\mathbf{r}) \) where \( \mathbf{k} \) is a vector lying in the Brillouin zone, consistent with the boundary conditions \( \exp(i\mathbf{k} \cdot \mathbf{L}) = 1 \), and \( \mathbf{L} \) is a dimension of the crystal.

\[
\left(-\frac{\hbar^2}{2m} \nabla^2 + \mathcal{V}(\mathbf{r}) - \varepsilon\right) \psi = 0, \tag{1.37}
\]

which remains the same after we have substituted \( \mathbf{r} + \mathbf{l} \) for \( \mathbf{r} \) in the operator that acts on \( \psi \).