Physics 489 S 04 Lecture 5
The Reciprocal Lattice (Ashcroft and Mermin, chapter 5)

1. Fourier Series for periodic function:
   For *any* property of a periodic system:
   If $f(x+T_n) = f(x)$ for all translations $T_n = na$, $n =$ integer,
   then
   $f(x) = \sum_G f_G e^{iGx}$, where $G = integer \times 2\pi/a$.
   Extends to any dimension:
   $f(\mathbf{r}) = \sum_{m_1,m_2,m_3} f(\mathbf{G}_{m_1,m_2,m_3}) e^{i\mathbf{G}_{m_1,m_2,m_3}\cdot\mathbf{r}}$, or $f(\mathbf{r}) = \sum_{\mathbf{G}} f(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}}$,

2. Definition of Reciprocal Lattice
   a. Bravais lattice of points in reciprocal space (k-space or G-space):
   $\mathbf{G}_{m_1,m_2,m_3} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3$
   b. Expressions for primitive vectors $\mathbf{b}_i$:
   $\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$
   Explicit forms in 1,2,3 dimensions
   c. Volume of primitive cell of reciprocal lattice $= (2\pi)^3/\Omega$, where $|omega =$ volume of primitive cell of real lattice.

3. Examples:

Real lattice	Reciprocal lattice
simple cubic	simple cubic
fcc	bcc
bcc	fcc
tetragonal ($\|a_3\| > \|a_1\|, \|a_2\|$)	tetragonal ($\|b_3\| < \|b_1\|, \|b_2\|$)
simple hexagonal	simple hexagonal (rotated)

4. Brillouin Zones:
   First Brillouin Zone (BZ) = Wigner-Seitz cell of Reciprocal lattice

5. Lattice planes:
   Miller indices: (h,k,l) denotes family of planes; {h,k,l} denotes set of equivalent (h,k,l)
   One-one correspondence: family of planes (h,k,l) to a reciprocal lattice vector **G** that is the shortest **G**-vector orthogonal to the planes
   Easier to use planes in some cases, e.g., to describe a plane of atoms that forms a surface
   In general, much easier to use reciprocal lattice to describe properties of periodic crystals