Recall: vectors and planes

\([uvw]\): find intercepts, clear fractions

- \([001]\)
- \([012]\)
- \([021]\)
- \([010]\)
- \([110]\)
- \([101]\)
- \([112]\)
- \([301]\)

\((0,0,0)\)
Recall: Miller index notation

For plane \((hkl)\): find intercepts, take reciprocal

Example: fcc unit cell
**Periodic surfaces (S&L, Ch. 2)**

- Surfaces can possess periodic translations that differ from bulk unit cell projection due
  - Adatoms
  - Reconstruction
  - Surface defects
  - Overlayer adsorption
- **Superlattice:** periodic structure of overlayers

**Surface unit cell**

The primitive unit cell is the simplest periodically repeating unit which can be identified in an ordered array. By translating a unit cell, the whole array can be constructed.
Example: simple cubic unit cell

Example: fcc unit cell
fcc unit cell

fcc unit cell: Distance between layers

\[ h = \frac{1}{2} a_o \]

\[ h = \frac{\sqrt{2}}{4} a_o \]

\[ h = \frac{\sqrt{3}}{3} a_o \]
Example: diamond

- fcc with every other $T_d$ hole filled
- Cubic fcc lattice with a two-atom basis:
  
  $C(0,0,0)$
  $C(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$

Diamond unit cell
Overlayer superlattices – matrix notation

To describe how an overlayer sits on a surface plane, we use the surface unit vectors to describe the superlattice, not the bulk unit cell projection.

\[ a' = m_{11}a + m_{12}b \]
\[ b' = m_{21}a + m_{22}b \]

\[ M = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \]

Example: fcc layers

\[ M = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \]
\[ M = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \]
\[ M = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \]
Primitive overlayers – Wood’s notation

\[ M = \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix} \]

- Possess no diagonal overlayers
- Abbreviated as “p” for primitive
- Can be expressed as \((m_1 \times m_2)\)

**Primitive superlattices**

- fcc (100) – (1x1)
- fcc (100) – (2x2)
- fcc (100) – (3x3)
Adsorbate sites can vary

fcc (110) – (2x2)

Rotated primitive superlattices

\[ a' = a + b \]
\[ b' = a - b \]
\[ M = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \]

But, if we rotate the unit cell by 45°, we can use a primitive notation:

\[ a' = \sqrt{2} a + 0 b \]
\[ b' = 0 a + \sqrt{2} b \]

\[ M = \begin{pmatrix} \sqrt{2} & 0 \\ 0 & \sqrt{2} \end{pmatrix} \text{R45°} = (\sqrt{2} \times \sqrt{2}) \text{R45°} \]
Non-primitive lattice

...or we can describe it as a centered superlattice:

Common superlattice structures
Notation of high-index surfaces

Terraces separated by steps

Next: terraces, steps, kinks, adatoms...