Notes:

- **Office hours:** Monday & Wednesday 11:30-12:30, Thursday 1PM.
- I sent **email** yesterday. If you didn't get my email let me know. (Or also let me know if you prefer a different email address than the one I used).

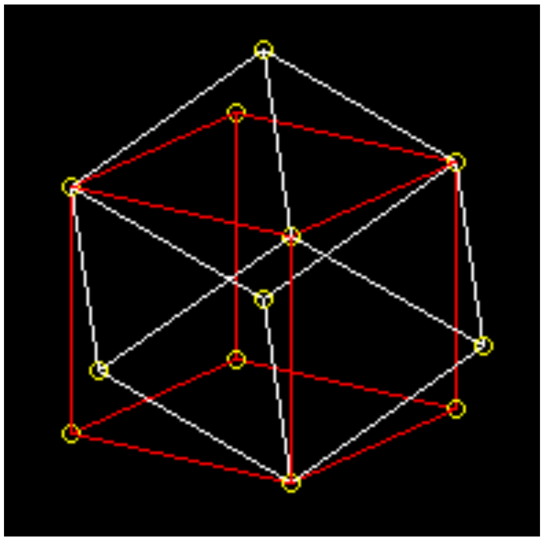
Reciprocal Lattice:

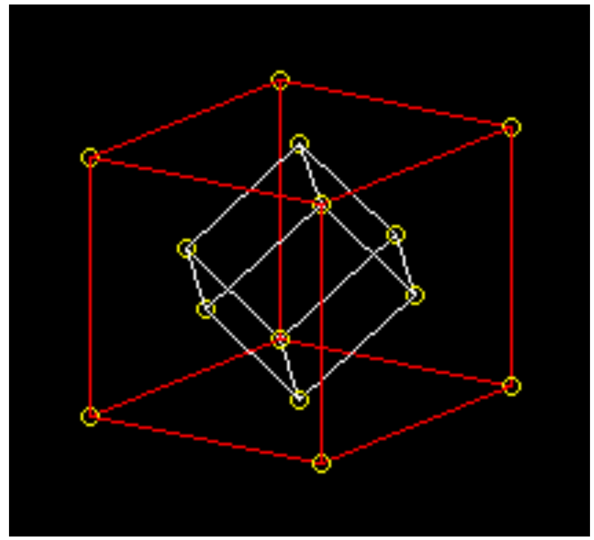
- **Composed of plane waves having symmetry of lattice:** $e^{i\vec{K}\cdot(\vec{r}+\vec{R})} = e^{i\vec{K}\cdot\vec{r}}$
- To construct: $\vec{K} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3$ with $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$
- **Find** (3D case): $\vec{b}_1 = 2\pi\dfrac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$ $\quad \vec{b}_2 = \dfrac{2\pi\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$ $\quad \vec{b}_3 = \dfrac{2\pi\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$

Cubic Bravais Lattice systems & primitive cells

From last time

white parallelpipeds: cell edges $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$





BCC (body center)
2 sites / cubic cell
Examples: Iron, Na

FCC (face center)
4 sites / cubic cell
Examples: Cu, Al, Ni, Silicon*, NaCl*, etc
*** These are FCC with basis**

Find: FCC lattice reciprocal is BCC lattice

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Results:

- Wavefronts of $e^{i\vec{K}\cdot\vec{R}}$ are Bragg planes (lattice planes);

  shows that $\dfrac{2\pi}{d}\hat{n}$ is a K vector; *h, k, ℓ* ⇔ *h, k, ℓ*
- Reciprocal lattice is itself a Bravais lattice; "dual" to direct lattice. Also reciprocal of reciprocal lattice = direct lattice.
- K vectors: k-space Fourier components of direct-space lattice.

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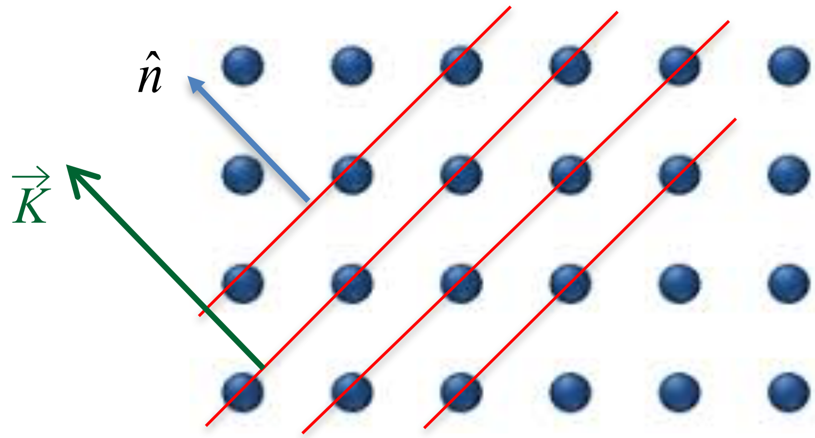

- Reciprocal lattice is itself a Bravais lattice; "dual" to direct lattice. Also reciprocal of reciprocal lattice = direct lattice.

- K vectors: k-space Fourier components of direct-space lattice (complete set).

$$n(\vec{r}) = \sum_{\vec{K}} n_{\vec{K}} \exp[i\vec{K}\cdot\vec{r}] \qquad n_{\vec{K}} = \frac{1}{V_{cell}} \int_{cell} d^3r\, n(r) \exp[-i\vec{K}\cdot\vec{r}]$$

Also: • Wigner-Seitz reciprocal cell = 1st Brillouin Zone. • Volume = $\dfrac{(2\pi)^3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}$