Scattering From Lattice with a Basis

- What does $\frac{d\sigma}{d\Omega dE}$ look like for a lattice with basis?

  - Still have $\frac{d\sigma}{d\Omega dE} \propto |M(\vec{q})|^2$

  - $M(\vec{q}) = \sum_{\alpha} \int d^3\vec{r}\; e^{-i\vec{q}\cdot\vec{r}}\, U_\alpha(\vec{r}-\vec{r}_\alpha)$

- α is atom label. For lattice with basis,

  ~ $\alpha \to \vec{R}, i$ ← basis index $i = 1, \ldots, k$

  ↑ Bravais lattice vector

  (k atoms in basis)

  ~ $\vec{r}_\alpha \to \vec{R} + \vec{c}_i$ ← basis vector for ith atom

  ~ $U_\alpha(\vec{r}-\vec{r}_\alpha) \to U_i(\vec{r}-\vec{R}-\vec{c}_i)$

$$M(\vec{q}) = \sum_{\vec{R}} \sum_{i=1}^{k} \int d^3\vec{r}\; e^{-i\vec{q}\cdot\vec{r}}\, U_i(\vec{r}-\vec{R}-\vec{c}_i)$$

$$\downarrow \quad \vec{r} \to \vec{r} + \vec{R} + \vec{c}_i \quad \text{(change of variables)}$$

$$= \sum_{\vec{R}} \sum_{i=1}^{k} e^{-i\vec{q}\cdot\vec{R}}\, e^{-i\vec{q}\cdot\vec{c}_i}\, U_i(\vec{q})$$

$$= \left[\sum_{i=1}^{k} U_i(\vec{q})\, e^{-i\vec{q}\cdot\vec{c}_i} \right] \sum_{\vec{R}} e^{-i\vec{q}\cdot\vec{R}}$$

$$= N \left[\sum_{i=1}^{k} U_i(\vec{q})\, e^{-i\vec{q}\cdot\vec{c}_i} \right] \sum_{\vec{Q}} \delta_{\vec{q},\vec{Q}}$$

↑ RL of $\{\vec{R}\}$ Bravais lattice

~~$|M(\vec{Q})|^2 \neq N^2 \sum_{\vec{Q}} \ldots$~~

$$\Rightarrow \boxed{|M(\vec{Q})|^2 = N^2 \sum_{\vec{Q}} T(\vec{Q})\, \delta_{\vec{q},\vec{Q}}}$$

$$\boxed{T(\vec{Q}) = \left| \sum_{i=1}^{k} U_i(\vec{Q})\, e^{-i\vec{Q}\cdot\vec{c}_i} \right|^2}$$

- $T(\vec{Q})$ is essentially $|S_{\vec{Q}}|^2$, where A&M call $S_{\vec{Q}}$ the geometrical structure factor. I will not use this terminology, since it conflicts with something else more commonly called the structure factor in condensed matter physics.

- For a monatomic crystal, $U_i(\vec{Q}) \to U_1(\vec{Q})$, and

$$T(\vec{Q}) = |U_1(\vec{Q})|^2 \left| \sum_{i=1}^{k} e^{-i\vec{Q}\cdot\vec{c}_i} \right|^2$$

Note: This is actually not free of assumptions, because symmetry does not always require $U_i(\vec{Q})$ to be the same for the same atom. For example, in the diamond structure, $U_i(\vec{Q})$ of one atom in the unit cell is the rotation of $U_i(\vec{Q})$ for the other. ~~However, if we treat each atom as~~

However, if most scattering happens very close to the nucleus, then we approximately have spherical symmetry, and all atoms have the same form factor.

- Most important physics:
  - $T(\vec{Q})$ or (some) makes Bragg peaks disappear that would otherwise be there, if lattice was just the underlying Bravais lattice.

Structure within unit cell $\Leftrightarrow$ Destructive interference that eliminates some Fourier components.

  - The (somewhat) arbitrary choice of Bravais lattice + basis does not affect the physics. For example, $M(\vec{q})$ is the same for BCC, whether viewed as a Bravais lattice, or as simple cubic lattice with basis. $T(\vec{Q})$ factor takes care of making sure this works out.