Condensed Matter Physics – FK7060, Jan. 23, 2018.

Lecture 3 – Crystal lattices

Reading

Ashcroft & Mermin, Ch. 4, pp. 64 – 82.

Content

- Bravais lattice, primitive vectors
- Coordination number
- Unit cell, Wigner-Seitz cell
- Lattice with basis, crystal structure
- Close packing
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Central concepts

- **Bravais lattice, primitive vectors**

  Periodic array of discrete points that is infinite and appearing *exactly* the same from any point in the array. The positions of the points in a 3D Bravais lattive are given by

  $$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

  where $\mathbf{a}_i$ are three vectors ("primitive vectors") not in the same plane and n_i take any integral values.

  Each point in the Bravais lattice takes a unit of one or more atoms (or ions) to form a crystal structure.

  The body-centered cubic (bcc) and face-centered cubic (fcc) structures can be described as cubic Bravais lattices with base units of 2 and 4 atoms, but are actually also Bravais lattices.

- **Coordination number**

  Number of nearest neighbors of a given lattice point. Simple cubic (sc): 6, bcc: 8, fcc: 12

- **Unit cell, Wigner-Seitz cell**

  A *primitive unit cell* is placed on each Bravais lattice point to fill all space. It, thus, contains one lattice point. It can be constructed in different ways.

  A *conventional unit cell* is placed on a subset of a Bravais lattice (the subset also being a Bravais lattice) to fill all space. Example: bcc = sc + conventional unit cell containing 2 points. The *lattice parameters* describe the size of the unit cell.

  A *Wigner-Seitz cell* is a primitive unit cell containing the space closest to the center of the cell, i.e., closer to that cell center than to the center of any other neighboring cell.

- **Lattice with basis, crystal structure**

  A *crystal structure* is a Bravais lattice with a *basis* of the same physical unit at each Bravais lattice point. The resulting structure does not need to be a Bravais lattice.

- **Close packing**

  Structures that pack spheres with highest possible density.

- **Examples of crystal structures**

  Simple cubic (sc): Cubic bravais lattice

  Body centered cubic: Bravaislattice equivalent to *sc* plus 2-point basis of $\mathbf{0}$ and $(a/2)(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$.

  Face centered cubic: Bravaislattice equivalent to *sc* plus 4-point basis of $\mathbf{0}$, $(a/2)(\hat{\mathbf{x}} + \hat{\mathbf{y}})$, $(a/2)(\hat{\mathbf{x}} + \hat{\mathbf{z}})$, and $(a/2)(\hat{\mathbf{y}} + \hat{\mathbf{z}})$. The fcc lattice is close-packed.

  Diamond structure: equivalent to *fcc* lattice with 2-point basis of $\mathbf{0}$ and $(a/4)(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$.

  Simple hexagonal structure (rare): Bravais lattice obtained by stacking two-dimensional, triangular nets directly above each other.

  Hexagonal closed-packed structure (hcp): equivalent to a simple hexagonal lattice with 2-point basis of $\mathbf{0}$ and $\mathbf{a}_1/3 + \mathbf{a}_2/3 + \mathbf{a}_3/2$, where

  $$\mathbf{a}_1 = a\hat{\mathbf{x}} \quad , \quad \mathbf{a}_2 = \frac{a}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}a}{2}\hat{\mathbf{y}} \quad \text{, and} \quad \mathbf{a}_3 = c\hat{\mathbf{z}}$$

  are the primitive vectors spanning the simple hexagonal lattice. The packing is *ideal* if $c/a = \sqrt{8/3}$.

  Sodium chloride structure: Described by an *fcc* lattice with a basis consisting of one type of ion at $\mathbf{0}$ and another type at $(a/2)(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$.

  Cesium chloride structure: Described by a *sc* lattice with a basis consisting of one type of ion at $\mathbf{0}$ and another type at $(a/2)(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$.

  Zincblende structure: Described by an *fcc* lattice with a basis consisting of one type of ion at $\mathbf{0}$ and another type at $(a/4)(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$.

  Tetragonal structures: Have three perpendicular, primitive lattice vectors, but only two of equal length.

  Orthorhombic structures: Have three perpendicular, primitive lattice vectors, all of different lengths.

  Monoclinic structures: As orthorhombic, but with distorted angle of face perpendicular to c-axis.

  Triclinic structure (rare): Has three primitive lattice vectors with no special relationships to one another.

  Rhombohedral structure, also called *trigonal*: Has three primitive lattice vectors of equal length making equal angles with one another (not taking any special values).

- **Classification of crystal systems (Ch. 7)**

  There are fourteen Bravais lattices of different symmetries. These are divided into seven different crystal systems. There are the three *cubic systems* (*sc*, *bcc*, *fcc*), the *tetragonal systems* (2 kinds), the *orthorhombic systems* (4 kinds), the *monoclinic systems* (2 kinds), a *triclinic system*, a *trigonal system*, and one *hexagonal system* (the simple hexagonal).

  Allowing any basis at each Bravais lattice point, it is possible to create 230 different symmetry groups, the 230 *space groups*.