Crystal Lattices
(Ashcroft/Mermin: chapter 4)

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Survey of the most important geometrical properties of periodic arrays in three-dimensional space
Bravais Lattice

Unit Cells

Crystal Structures
Bravais Lattice

Unit Cells

Crystal Structures
Bravais Lattice – Definition

Definition of Bravais Lattice

a) Infinite array of discrete points with an arrangement and orientation that appears exactly the same, from whichever of the points the array is viewed

b) Consists of all points with position vectors \( \mathbf{R} \) of the form

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

(\( \mathbf{a}_i \) linear independent, \( n_i \) integer number)

- The \textit{primitive vectors} \( \mathbf{a}_i \) \textit{generate} or \textit{span} the lattice.
- There are infinitely non-equivalent choices for the set \( \{ \mathbf{a}_i \} \).
- It is not always easy to perceive the existence of such a set.

Definition of coordination number

Number of points in a Bravais lattice that are closest to a given point (nearest neighbours)
Bravais Lattice – Examples

a 2D Bravais lattice (a net)

- $P = a_1 + 2a_2$
- $Q = -a_1 + a_2$

honeycomb (not a Bravais lattice)

- view from $P$ and $Q$ different than from $R$
Bravais Lattice – Examples

several possible choices of pairs of primitive vectors
Bravais Lattice – cubic

simple cubic lattice
coordination number 6

primitive vectors

\[ a_1 = a \hat{x} \]
\[ a_2 = a \hat{y} \]
\[ a_3 = a \hat{z} \]

body-centered cubic (bcc) lattice
coordination number 8
Bravais Lattice – body centered cubic (bcc)

primitive vectors for the bcc Bravais lattice

- \( \mathbf{a}_1 = a\hat{x} \)
- \( \mathbf{a}_2 = a\hat{y} \)
- \( \mathbf{a}_3 = a/2(\hat{x} + \hat{y} + \hat{z}) \)
- \( P = -\mathbf{a}_1 - \mathbf{a}_2 + 2\mathbf{a}_3 \)

more symmetric primitive vectors

- \( \mathbf{a}_1 = a/2(\hat{y} + \hat{z} - \hat{x}) \)
- \( \mathbf{a}_2 = a/2(\hat{z} + \hat{x} - \hat{y}) \)
- \( \mathbf{a}_3 = a/2(\hat{x} + \hat{y} - \hat{z}) \)
- \( P = 2\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3 \)
Bravais Lattice – face centered cubic (fcc)

- Coordination number 12
- $a_1 = a/2(\hat{y} + \hat{z})$
- $a_2 = a/2(\hat{z} + \hat{x})$
- $a_3 = a/2(\hat{x} + \hat{y})$
- $P = a_1 + a_2 + a_3$
- $Q = 2a_2$
- $R = a_2 + a_3$
- $S = -a_2 + a_2 + a_3$

An enormous variety of solids crystallize in the bcc or fcc form
Bravais Lattice

Unit Cells

Crystal Structures
**Definition of Primitive Unit Cell**

Volume of space that, when translated through all the vectors in a Bravais lattice, fills all of space without overlapping itself or leaving voids

- It is not unique

Obvious choice: all points $\mathbf{r}$ with

$$
\mathbf{r} = x_1 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_3 \mathbf{a}_3, \quad 0 \leq x_i \leq 1
$$

- The numbers specifying the size of a unit cell are called *lattice constants*
Conventional Unit Cell

Definition of Conventional Unit Cell

A region that fills space without any overlapping when translated through some *subset* of the vectors of a Bravais lattice

- Usually chosen larger than the primitive unit cell and to have the required symmetry

bcc unit cells

fcc unit cells
**Wigner–Seitz Primitive Cell**

**Definition of Wigner–Seitz Cell**

The region of space around a lattice point that is closer to that point than to any other lattice point

- Primitive cell with full Bravais lattice symmetry
- Generalization to any set of discrete points: Voronoy polyhedron

![bcc Wigner–Seitz cell](image1)

![fcc Wigner–Seitz cell](image2)
Bravais Lattice

Unit Cells

Crystal Structures
Crystal Structure – Definition

Definition of Crystal Structure

Identical copies of the same physical unit, called the basis, located at all points of a Bravais lattice

- A physical crystal can be described by giving its underlying Bravais lattice, together with a description of the arrangement of atoms within a particular primitive cell
- One can also describe a Bravais lattice as a lattice with a basis by choosing a conventional unit cell with a basis of more than one point

bcc: conventional unit cell with two-point basis
fcc: conventional unit cell with four-point basis
Diamond Structure

The diamond lattice

- consists of two interpenetrating fcc Bravais lattices which are
- displaced along the body diagonal of the cubic cell by one quarter the length of the diagonal
- is not a Bravais lattice

- coordination number 4
- fcc lattice with two-point basis $0, \ (a/4)(\hat{x} + \hat{y} + \hat{z})$

Zincblende structure

- Equal numbers of cations and anions distributed on a diamond lattice
- Each ion is coordinated by 4 counterions
Hexagonal Close-Packed Structure (hcp)

Underlying structure

- a simple hexagonal Bravais lattice given by
- stacking 2D triangular nets directly above each other

- primitive vectors: $\mathbf{a}_1 = a\hat{x}$, $\mathbf{a}_2 = a/2\hat{x} + \sqrt{3}a/2\hat{y}$, $\mathbf{a}_3 = c\hat{z}$
- Direction of stacking ($\mathbf{a}_3$) is known as $c$-axis
Hexagonal Close-Packed Structure (hcp)

The hexagonal close-packed structure (hcp)

- consists of two interpenetrating simple hexagonal Bravais lattices, displaced from one another by $a_1/3 + a_2/3 + a_3/2$
- ideal ratio $c/a = \sqrt[3]{8/3} \approx 1.63$, other ratios possible
- is not a Bravais lattice
- ranks in importance with bcc and fcc Bravais lattices
- about 30 elements crystallize in the hcp form

hcp packing (…ABABABAB…)
Other Close-Packing Possibilities

...back to fcc

There are infinite many possibilities for close packing

- Certain rare earth metals take on a structure of the form (...ABACABACABAC...)  

bcc is not close packed!
Sodium Chloride Structure

- Equal number of cations and anions placed at alternate points of a simple cubic lattice
- Each ion is coordinated by 6 counterions
- fcc Bravais lattice with two-point basis
  \[ 0, \ (a/2)(\hat{x} + \hat{y} + \hat{z}) \]
in conventional cubic cell
Cesium Chloride Structure

- Equal number of cations and anions placed at the points of a bcc lattice
- Each ion is coordinated by 8 counterions
- Simple cubic Bravais lattice with two-point basis \(0, (\frac{a}{2})(\hat{x} + \hat{y} + \hat{z})\) in conventional cubic cell
A comparison

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<tr>
<th>structure</th>
<th>coord. no.</th>
<th>space-filling</th>
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<tbody>
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<tr>
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<tr>
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<td>0.52</td>
</tr>
<tr>
<td>diamond</td>
<td>4</td>
<td>0.34</td>
</tr>
</tbody>
</table>

- Reasons for taking up different crystal structures...
Conclusions

We have described

- the *translational symmetry* of crystal lattices in *real physical space*

We will subsequently hear about

- translational symmetry in *reciprocal space* (chapter 5)
- some features of the *rotational* symmetry (chapter 7)