

Science of Lattices and Crystals

Science

Before I get started: These two modules give a first idea about lattices and crystals *without* all the formal stuff coming up here:

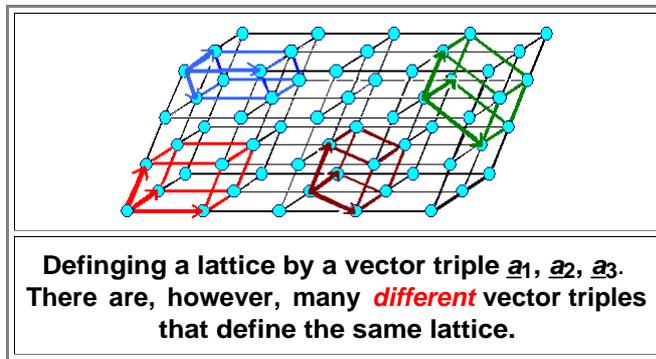
- [Crystal Models](#). You learn how you have to look at all these schematic figures of crystals and why you can't take them at face value.
- [Lattice and Crystal - Simple View](#). The basics without math.

Bravais Lattices

Any crystal lattice can be described by giving a set of three **base vectors** \underline{a}_1 , \underline{a}_2 , \underline{a}_3 . A lattice is formed by generating an infinity of **translations vectors** $\underline{T} = u\underline{a}_1 + v\underline{a}_2 + w\underline{a}_3$ with $u, v, w, =$ integers. The end points of all possible translations vectors define the lattice as a periodic sequence of points in space.

If you have some lattice and move it by any translation vector you care to construct, you have *exactly* the same lattice once more. In other words: crystal lattices show a **translation symmetry**! For a long time, the words "*crystal*" and *translation symmetry* were seen as obvious synonyms - until the discovery of [quasi-crystals](#) in 1982!

Unfortunately, one and the same lattice can be defined by many different sets of vector triples as illustrated right below.



It is far easier to use some *special* lattices instead of just one general type. The thing to do is to go for **symmetries** as the distinguishing criterion. That's what **Bravais** did, showing that with 14 **Bravais lattices** all possible cases can be represented. All material scientists know that "magic" number **14** but very few know how it is derived. I don't know details either but I know it is an exercise in set theory.

Note that a **lattice** is a *mathematical* construct, a succession of (infinitely small) mathematical points in space. A perfect drawing of such a lattice thus would show nothing at all. Instead of *points*, I use little blue spheres here. They are connected with lines but *only* to "guide the eye".

These blue spheres are *not* representing atoms when a *lattice* is shown. More about figures to lattices and crystals in [this link](#).

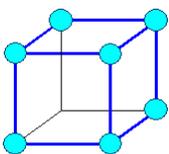
If one wants to make a **crystal**, one assigns a so-called **base of atoms** to a lattice point. If that base happens to consist of just *one* atom or element, we make an **element crystal**. A *schematic* figure of such a crystal with one atom per lattice point then looks exactly like the *schematic* representation of a lattice, causing no end of confusion. It is nevertheless something *completely different*; see below.

Note that mother nature has not made a cubic primitive *element* crystal.

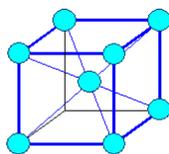
Bravais Lattices and Their Parameters

Cubic

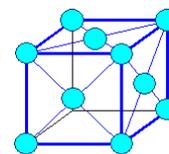
$$\underline{a}_1 = \underline{a}_2 = \underline{a}_3 = \underline{a} = \text{lattice constant} \quad \alpha = \beta = \gamma = 90^\circ$$



cubic primitive



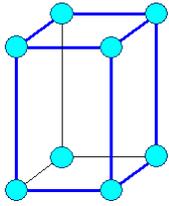
cubic body centered (bcc)



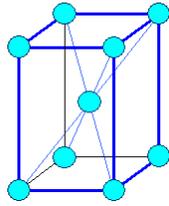
cubic face centered (fcc)

Tetragonal

$$a_1 = a_2 \neq a_3 \quad \alpha = \beta = \gamma = 90^\circ$$



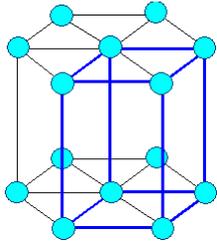
tetragonal primitive



tetragonal body centered

Hexagonal

$$a_1 = a_2 \neq a_3 \quad \alpha = \beta = 90^\circ, \gamma = 120^\circ \quad \text{Typical: } a_3 = c$$

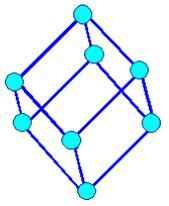


Hexagonal (hex)

(expanded to show hex symmetry)

Rhombohedral or Trigonal

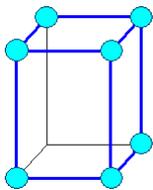
$$a_1 = a_2 = a_3 \quad \alpha = \beta = \gamma \neq 90^\circ$$



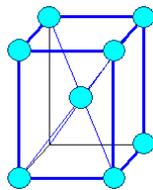
rhombohedral

Orthorhombic

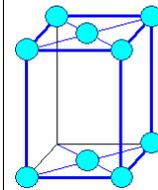
$$a_1 \neq a_2 \neq a_3 \quad \alpha = \beta = \gamma = 90^\circ$$



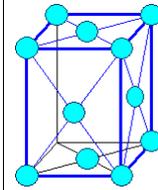
orthorhombic primitiv



orthorhombic body centered



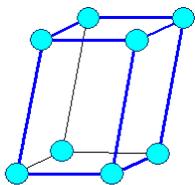
orthorhombic base face centered



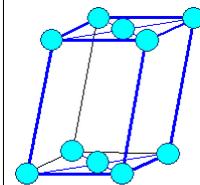
orthorhombic face centered

Monoclinic

$$a_1 \neq a_2 \neq a_3 \quad \alpha = \beta = 90^\circ, \gamma \neq 90^\circ$$



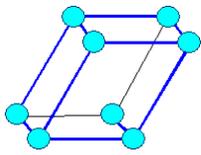
monoclinic primitive



monoclinic base face centered

Triclinic

$$a_1 \neq a_2 \neq a_3 \quad \alpha \neq \beta \neq \gamma \neq 90^\circ$$



triclinic

Bravais lattices

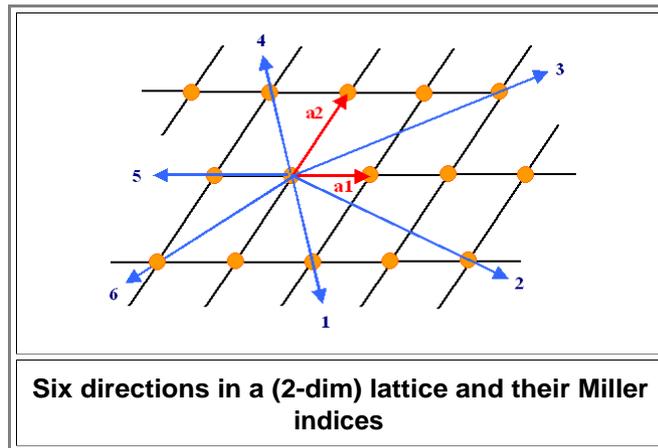
(on occasion only "visible" lattice points (= blue circles) are shown)

Describing Directions and Planes by Miller Indices

Working with lattices and crystals produces rather quickly the need to describe certain directions and planes in a simple and unambiguous way. Stating that an elemental face-centered cubic crystal can be made by assigning one atom to any lattice point found on "that plane that runs somehow diagonally through the unit cell" just won't do it. So **William Hallowes Miller** invented a system with a lot of power for doing that in 1839. What we do is to describe any direction or any plane by *three integer numbers*, called **Miller indices**.

How to derive the Miller indices of a certain direction or plane is easy. Here is the recipe for directions (in 2 dimensions for simplicity); the figure below illustrates it:

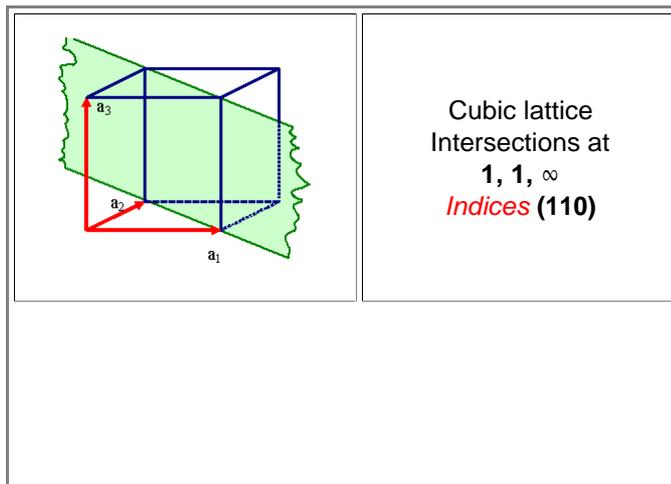
- Start the desired direction from the origin.
- Express the direction as a vector given in integer multiples u, v, w of the base vectors.
- Make sure the three integers have the smallest possible value.
- Write the direction as $[u \ v \ w]$ or $\langle u \ v \ w \rangle$ (we won't concern us here with the subtleties involved in using two kinds of brackets).
- Negative integer values are written with a dash on top of the number instead of the conventional "-" sign. (not possible in simple HTML)



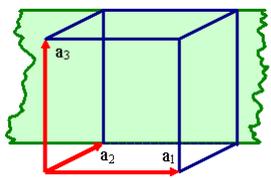
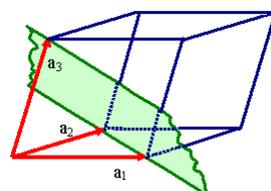
Six directions in a (2-dim) lattice and their Miller indices

Getting Miller indices for planes is a bit more involved. Here is how it's done; the figure below gives examples:

- Put the origin *not* on the plane but on a neighboring plane.
- Find the intersection points $h', k',$ and l' of the plane with the (extended) base vectors. If there is none, the value is ∞ .
- Form the reciprocal values of $h', k',$ and l' and call them $h, k,$ and l . If, for example, $h' = \infty$, you have $h = (1/h') = 0$.
- The Miller indices of the plane to be indexed then are $\{hkl\}$ or (hkl) .



Cubic lattice
Intersections at
1, 1, ∞
Indices (110)

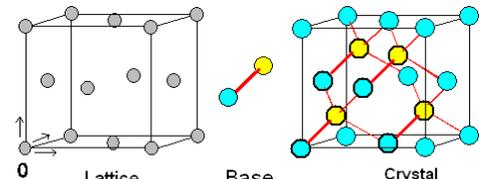
	<p>Cubic lattice Intersections at $\infty, 1, \infty$ Indices (010)</p>
	<p>Triclinic lattice Intersections at $1, 1, 1$ Indices (111)</p>
<p>Miller Indices for Planes</p>	

- If you wonder why this slightly awkward procedure was adopted, the answer is easy: You can use the Miller indices directly in a lot of equations needed for calculating properties of crystals.

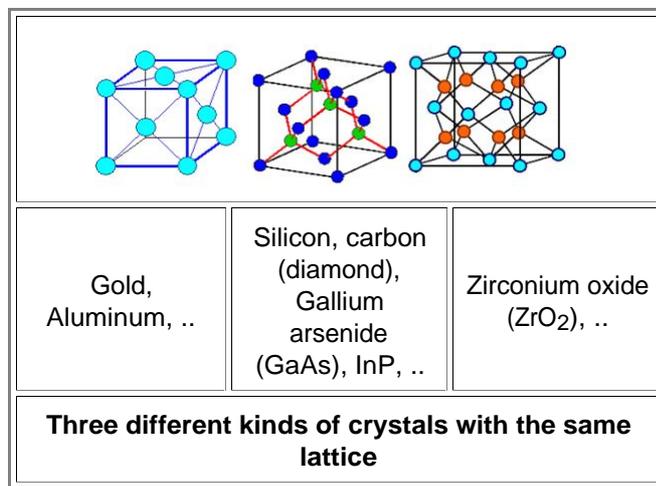
From Lattice to Crystal

Any crystal can be made following this easy recipe:

- Pick a Bravais lattice
- Pick a base, a collection of atoms in a fixed spatial relation (similar and often but not always identical to a molecule of the substance).
- Put the base in the same way on any lattice point.


<p>How to make a diamond-type crystal</p>
<p>The yellow atom of the base is only shown if it is found inside the unit cell</p>

- The example above shows how to make a crystal of the diamond type. The base consists of two atoms. In the coordinate system of the lattice unit cell (indicated by arrows), the two atoms have the coordinates $(0,0,0)$ and $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$.
If the two atoms are of the **same** kind, e.g. silicon, (Si), germanium (Ge), or carbon (C), you get a silicon, germanium or diamond crystal.
If the atoms are **different**, e.g. from [group III](#) or [group V](#) of the [periodic table](#), you get most of the compound semiconductors like gallium arsenide (GaAs), or indium phosphide (InP).
- This looks simple. It is not. It's the point where things get difficult and confusing. Ask yourself for any still simple crystal: how many atoms are there to a lattice plane? How many atoms are in a base?
Below are three **crystals**, all have an fcc lattice. Different colors of the circles may or may not denote different atoms. Can you figure out the bases? If you can, you're ahead of my average third-term student.



One last thought: Crystals in a general sense, meaning an arbitrary base arranged in a periodic way, can be found everywhere; here is an example:

