Script Unit 2.5

Welcome back - we now want to discuss the centering of cells more deeply.

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Well, we already know that there are 7 crystal systems. And if the lattice points are only at the corners of the unit cell then it is a primitive unit cell. In the last unit we learned that it can be advantageous if we add additional lattice points to the unit cell - the symmetry of course will not change, but the metric of the unit cell changes towards a better representation of the underlying symmetry of the lattice.

We will see, that if we allow to add further lattice points we get 7 more lattice types - giving 14 in total, leading us to the Bravais lattice - as a reminder: we do this, because we want to find the best representative for our crystal system, for the symmetry of the crystal system.

But let’s see firstly, what different kind of centerings exist. The primitive unit cell corresponds to no centering, it is not centered. The next possibility is, that there is one additional lattice point at one face of the unit cell - conventionally, it is the C-face, that is the plane that is spanned by the a- and b- lattice vector; it also can be the A or B-face in a non-conventional setting.

The next variant is the body-centering, in which an additional lattice point is placed exactly in the center of a unit cell, the symbol for this kind of centering is “I”, derived from “inside”. And, finally, the last possibility is, that there are additional lattice points at all faces, but not inside the unit cell - and the respective symbol is “F”.

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Let’s now examine how many lattice points belong to one unit cell depending on the given centering.

Well, if we take the primitive unit cell, we have 8 lattice points - one at every corner of the unit cell - and every lattice point belongs to 8 unit cells simultaneously - this means every lattice point belongs to one eighth of one unit cell - and 8 times one eighth is equal to one.

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In the case of the single-side face centering we have 8 lattice points at the corners of the unit cells and we have 2 points at faces - lattice points at faces belong to two unit cells simultaneously - this means the lattice points at the faces belong to one half to each unit cell - and this gives in the end 2 lattice points per unit cell in total.
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Regarding the I-centering we have 8 times one eighth for the lattice points at the corner and the additional lattice point inside the unit cell, in the center of the unit cell, which belongs, of course, only to one unit cell - so we have 2 lattice points or formula units per unit cell.

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And finally, in the case of F-centering we have 8 times one eighth lattice points at the corners and 6 times one half for all the lattice points at the faces - giving 4 lattice points in total per unit cell.

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Okey, in principle we have 4 kind of centerings, here they are shown again in an overview, the primitive non-centered case, the single-sided face-centered unit cell, the body-centered case and the all-side face-centered unit cell.

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I mentioned earlier, that there are 7 primitive lattices and if we account for centerings that there are 7 more lattice types - 14 in total - but this is not understandable at first sight - if we have 7 crystal systems and 4 kind of centerings, then the total number of different cells including centerings should be 28, not only 14. What is the reason for that?

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On the following slide all 14 types of unit cells are depicted synoptically. The crystal systems build the columns of this table-like overview, the type of centering the rows. Obviously, not for all of the crystal systems each type of centering exist, there are empty positions.

For the triclinic system for instance, only the primitive lattice and no centering exist. For the monoclinic system the primitive and the single-side face centered lattice types are conceivable, the orthorhombic crystal system exists in all variants of centering and so on.

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It was Auguste Bravais - a French physicist, crystallographer and universal scholar who could show in 1848 that only 14 principally different lattice types exist in three dimensions. The reason for that is twofold:

Firstly, some of the 28 that are conceivable in principle are redundant, meaning that certain lattice types can be mutually converted into each other - and this means simply that they do not constitute a lattice type of their own.
The second reason is that some of the centerings are not compatible with the symmetry of the crystal system. Let's have a look at an illustration for each of the two reasons:

**Slide 11**

Well, we have the primitive monoclinic cell and it is indeed allowed to build such a I-centered monoclinic unit cell, but this can also be described by a C-centered cell as shown here in red, so we do not need the I-centered variant. This was an example for redundancy.

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Now we cover a different case, namely in the cubic system - an all-face centered unit cell is one of the 14 unique Bravais lattices - but does also a C-centered cubic lattice exist?

No, this is not the case, because this would be incompatible with the symmetry of the cubic system - in the primitive cubic system the lattice vectors have all the same length $a$ -

But here the distances between equivalent lattice points are different - let’s look at this scheme - we have no centering on this face - this means the distance between these 2 points is $a$ - as it must be the distance between these 2 points linked by this red line, but what about this length? It is not $a$ - instead it is the square root of 2 divided by 2 times $a$ - this can be derived by the Pythagoras’ theorem.

So it turns out that this C-centered cell is not compatible with the cubic system, in fact it is a primitive tetragonal cell shown here in red.

**Slide 13**

Now we know the reasons why in this table not all centerings are listed - symmetry incompatibilities and redundancy -

There is one issue left with this table and this is the funny R-centering, which we do not understand yet - we will cover this in an extra unit - but for this, we need to introduce fractional coordinates - this will be done in the next unit.