Script Unit 2.8

In this unit we want to discuss the hexagonal crystal system in more detail.

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The hexagonal crystal system is a bit challenging to manage, a little less clear than the others, some even believe that the hexagonal system was invented by the devil - as a scientist I do not believe in anything but I would agree that the hexagonal system - although very beautiful - is indeed a bit complicated.

As a prerequisite I want to briefly introduce what a symmetry operation is. This is in slight anticipation of the next chapter, in which we will deal with all kind of symmetry operations in full length - but for now let's focus on the quintessence what a symmetry operation is.

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Well, a symmetry operation can be understood as follows:

Take an arbitrary object, for instance, this cube - then we will shut our eyes and then someone will do something with the cube, a geometric operation - for example a rotation by 90 degrees - if the operation, the transformation is finished, then we are allowed to open the eyes again - and if we can't recognize that something was done to this object, then it was a symmetry operation - the final state of this cube is indistinguishable!

Here, we carried out a rotation by 90° degrees and the respective symmetry element is a 4-fold axis of rotation.

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Inversely, if we take this cube, in which one face is decorated with this face and if we then rotate the cube along this axis by 90 degrees then we end up with this configuration - clearly, this is not a symmetry operation. Now we are ready to investigate a few details of the hexagonal crystal system.

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Here, you see again a hexagonal prism - and one third of it is the primitive hexagonal unit cell, the basal plane has edges of identical length a equals a and c is different and the angle here is 120 degrees. And if we look from above we see this projection - the lattice points of one unit cell are drawn here as blue circles.

And now we want to answer these three questions:
First: in which way are hexagonal unit cells assembled correctly?

Second: to how many unit cells does the central atom (1) belong?

And third: where is the 6-fold axis of rotation located?

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The first question: how to assemble hexagonal unit cells.

Well, actually there is always only one way to build a whole crystal structure by assembling unit cells, regardless of the crystal system, and this is to translate the unit cell in all 3 directions -

You might think, Frank, we already know that, what's the point? - Yeah, I understand this, but I wanted to point out the relationship between this primitive unit cell, which does not really look like something hexagonal and the hexagonal shape that is associated with the term “hexagonal” crystal system.

If we translate our unit cells we get something like this - if we now sketch-in the hexagonal shape of a prism, then we see that this is not composed of three unit cells as one would think at first sight. One might think that it is composed of these three cells, that are rotated and then assembled - but: rotation is not allowed - it is against the translation principle.

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Instead, the hexagon is composed of these two complete primitive unit cells and two halves of these primitive cells!

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The second question: to how many unit cells does this central atom or lattice point belong?

Well, why I am asking this? Because of this potentially confusing hexagon! Perhaps some of you think the answer is three - because of this pattern, which can be thought of being composed of these three cells.

Some of you might already take into account that this drawing is only a projection onto 2 dimensions and that we have to include the third dimension and therefore the correct answer is may be 6 ..!?

But the correct answer is of course 8! We have 4 neighboring unit cells in the 2-dimensional plane and 4 more if we extend this into three dimensions! Remember that all unit cells are parallelepipeds! A lattice point at the corner always belongs to 8 unit cells, regardless of the specific crystal system we consider.
If this was already clear to you - even better!

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The last question: the hexagonal crystal system is characterized by its 6-fold rotational symmetry - and the question is, where is this corresponding axis of rotation located?

Well, intuitively one might be inclined to place it at the center of the unit cell.

Let’s explore, if this is the case - we rotate the unit cell stepwise by 60 degrees around this axis… 10, 20, 30, 40, 50, 60…[Slide 10 to 13]

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Obviously, the final unit cell is not congruent with the starting position, this means: this was not a symmetry operation.

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The solution to this riddle is that the axis of rotation is located at one of the lattice points - at the corner of the unit cell!

If we now carry out the rotation by 60 degrees we end up with this pattern, this lattice point is transformed into this, this into that and this one comes over here, while the lattice point which coincides with the axis of rotation remains at its position.

You might think, that this is just a trick, because this point here belongs already to the neighboring cell - but the crystal actually does not care!

It does not matter because of the translational principle, because we are dealing with an endless, an infinite lattice - and remember a lattice is defined by the circumstance that every point of a lattice has the same surroundings - so, translation [in amounts of whole unit cells] is something that is not ‘detectable’, it has no impact.

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The hexagonal symmetry is easier to recognize if we take a larger part of the crystal lattice - now it is evident that this lattice does indeed possess hexagonal symmetry.
In particular if we wipe out these edges - remember a lattice is… FRANK! okey okey, you understood...and we will stop here for now!