Higher-Dimensional Structure Evaluation of the Aperiodic Structures Er_3Ru_2, $Y_{44}Ru_{25}$ and $LaRu_x$

The Er_3Ru_2 structure has been solved with superspace formalism and presence of superstructure has been proven in the other structures.

This thesis has answered the question; are the Er_3Ru_2, $Y_{44}Ru_{25}$ and $LaRu_x$ crystal structures aperiodic in three-dimensions and therefore better described in higher dimensions?

The short answer to the question above is yes! All three crystal structures can most likely be better described in four-dimensions.

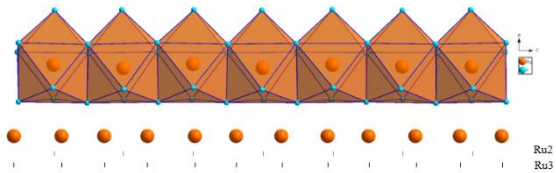
Investigating the crystal structure of compounds is vital in understanding how intrinsic properties such as magnetism and superconductivity arises and is of course of a general interest to the scientific community.

So why then is this higher-dimensional formalism required?

A distinctive property of crystalline materials is long- as well as short-range order in the atomic or molecular dimensions. A macroscopic single crystal can be built up by periodically translating the basic unit of the crystal, the unit cell, in three dimensions. However there is of course exceptions, being the aperiodic crystals. These crystals lack the translational symmetry of ordinary crystals, the periodicity is lost.

There are several things that can cause this loss of periodicity. Examples are interactions between atoms which distorts atoms from their original atomic positions or two interpenetrating subsystems which interacts with each other. This phenomenon can be visualized in figure 1.

Figure 1. Aperiodicity of two ruthenium atoms in the c-axis.



Here we can see that positions of the Ru atom inside the geometric shape never truly coincides with other ruthenium atom, the periodicity is lost. Just like the metric and imperial units on a ruler only coincides on the first marking.

Another analogy would be to consider an infinite row of seats with big boned occupants that spill over to adjacent seats. The first occupant will be seated in the first seat but the adjacent occupant will have to move a little further to the side of the respective seat and so on. If the first occupant are considered to belong to the first seat, the second occupant to the second seat and so on it's evident that the occupants will move further and further away from its equivalent seat as we move along the row.

It's this atomic perturbation that causes the aperiodicity of the structure which demands an additional dimension, modulation vector, in order to restore the translational symmetry of the structure.

In this thesis the Er_3Ru_2 structure was solved with the superspace formalism, the structure solution resulted in the non-centrosymmetric super-space group *X3 (00γ)0* with $a = b = 13.893$ (4) Å, $c = 4.0005$ (12) Å $q = 1.572$ c*. Additionally strong evidence of superstructures in the $LaRu_x$ and $Y_{44}Ru_{25}$ could be concluded, however these structures were not solved with the superspace formalism in this thesis and are considered future work.