Detecting defects using X-Ray diffraction in stuffed $Yb_2Ti_2O_7$

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Abstract

The main goal of this project is to determine a new way to detect defects within Ytterbium titanate by using X-Rays. The first step was to perform a standard X-Ray diffraction experiment, this produced expected results, however on could not see any diffuse scattering on hkl projections. The next step was to then try a new technique. Single shot diffraction was trialled as a potential method and indeed did show the diffuse scattering patterns. Finally, to compliment the single shot diffraction, a python script was written to calculate the hkl values at a given point on the single shot diffuse scattering and to compare with experiment.

Previous research

This experiment is a follow on from the paper by Bowman et al [1] in which neutrons were used to detect diffuse scattering. The difference between the Oxygen depleted and stuffed forms of Ytterbium titanate can be seen in Figure 2.

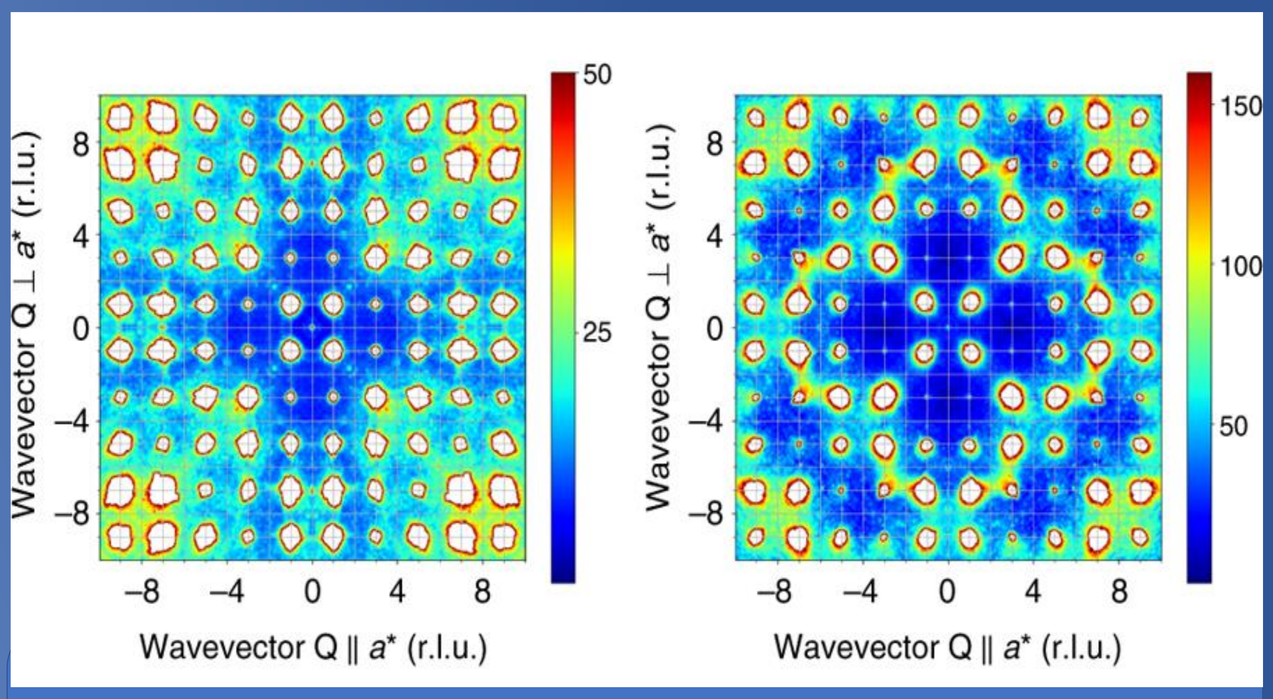

Figure 1: Results from Bowman et al [1]. These are two neutron scattering patterns for an Oxygen depleted (left) and stuffed form (right) of Ytterbium titanate.

X-Ray diffraction

The standard X-Ray diffraction experiment yielded predictable result, the projection onto the hk0 plane can be seen Figure 2. Here, the loss of any potential diffuse scattering an be seen in the variation in background, caused by the stitching together of multiple frames. This means that any of the broader, lower intensity peaks caused by diffuse scattering will be lost in the background.

After the standard diffraction experiment, the data was pulled into a refinement program. Here it was found that it was possible to refine on the occupation of the Titanium-Ytterbium site. In addition, the position of the Oxygen was found to be in close agreement with what was found by Bowman et al [1]. However, it was not possible to accurately refine on the occupation of the same Oxygen. Any attempt to do so lead to unphysical results.

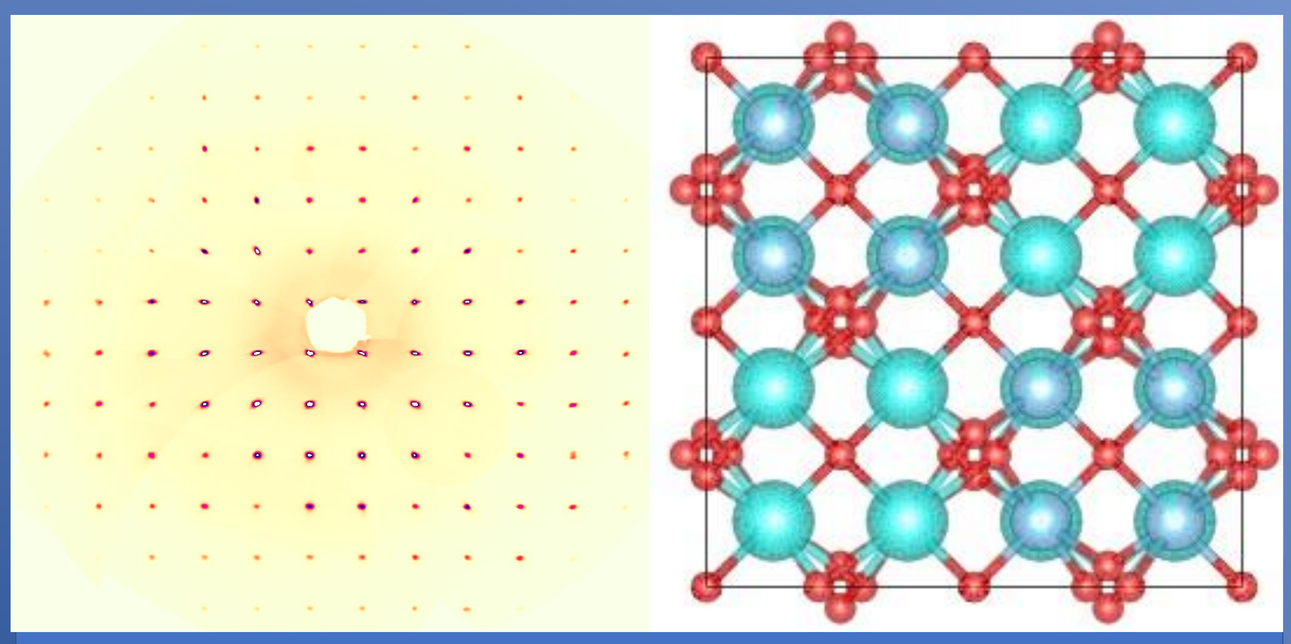

Figure 2: A projection across the hk0 plane (left). The discoloration around the central peaks is due to variation in absorption. The right displays a side on view of the structure of the crystal.

Single shot diffuse scattering

The new method trialled for attempting to detect defects was single shot diffraction. This involved looking at a single frame and trying to see if there is any evidence of diffuse scattering. As can be seen below on Figure 3, there is evidence of diffuse peaks being present within the frames. These can be spotted by there less sharp and broader nature.

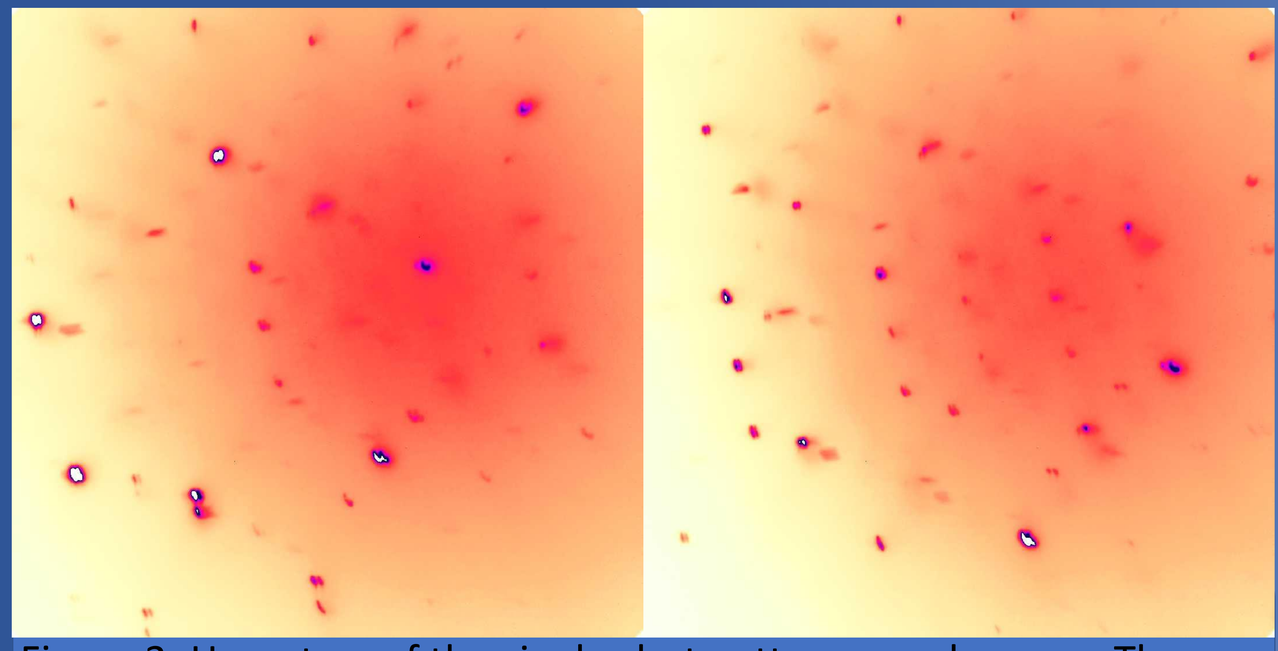

Figure 3: Here, two of the single shot patterns can be seen. The diffuse peaks can be seen on both frames as being broader and less sharp.

Python Simulation

The Python code written for this report aimed to predict the hkl values taken at each point of figure 3. This was done by implementing a series of rotations onto the lattice vectors and also adjusting for corrections in the detector to determine the value taken at each XY-coordinate (a full outline of the method can be found here [2]). This was found to be reasonably accurate.

Conclusions

In conclusion, the main aim was to determine new ways to detect defects in Ytterbium titanate. To that end, it was a success, with the single shot diffraction method showing diffuse scattering. However, the X-Rays do have a limted accuracy when compared to neutrons. Whilst the occupation on the Titanium-Ytterbium site was in agreement with the nominal value, the changes of occupation of one of the Oxygen atom was not detected.

References

1 Bowman et al, Role of defects in determining the magnetic ground state of Ytterbium titanate. Nature Communications, 10(1):637, 2019.

2 W. R. Busing and H. A. Levy. Angle calculations for 3- and 4-circle X-ray and neutron diffractometers. Acta Crystallographica, 22(4):457–464, Apr 1967.