Rare-earth Ion Doping of $CaWO_4$ for Quantum Information Processing

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PARADIM Research Experience for Undergraduates

Introduction

As quantum computing develops there is a need for qubit materials that possess long spin coherence times and sharp optical transitions[1]. Rare-earth (RE) ions like Er^{3+} have been found to exhibit these qualities as well as the potential for quantum transduction from microwave to optical signals[2]. To harness their qubit properties, the RE ions must be doped into a crystal lattice host material. This project focused on doping fifteen RE ions into a calcium tungstate lattice. The samples were then characterized for applications in quantum information processing.

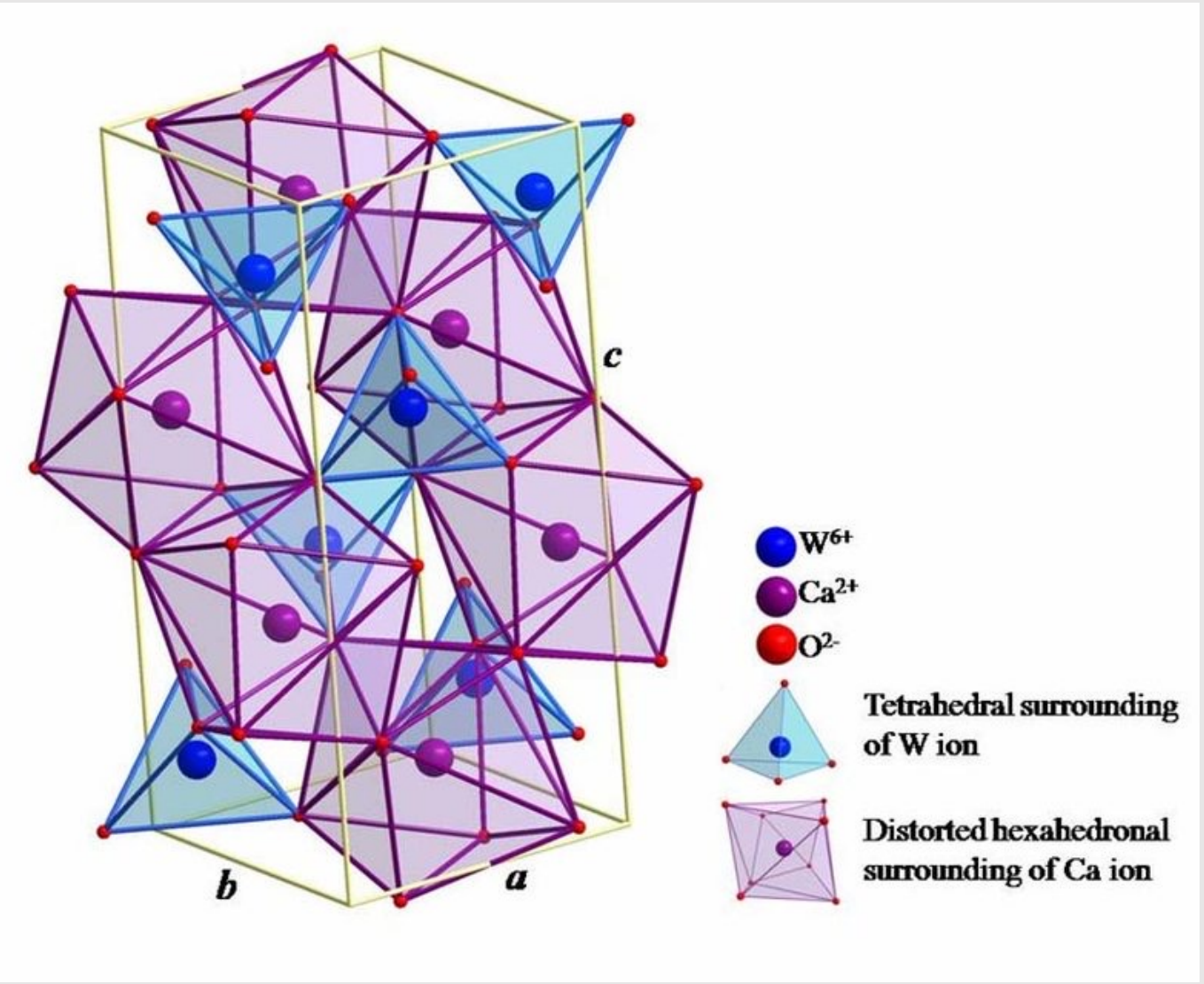

Fig 1. $CaWO_4$ unit cell from Abozaid R. M., et. al.

Methods

Each rare-earth oxide was combined with calcium carbonate and tungsten(VI) oxide using a mortar and pestle. A sample of 0.5%, 1%, and 5% doping concentration was synthesized for each of the fifteen rare-earth oxides used.

$$Ln_2O_3 + CaCO_3 + WO_3 \longrightarrow Ca_{1-x}Ln_xWO_4$$

The samples were then heated in a box furnace to 1050 °C. Once cool, the polycrystalline material was reground before performing XRD analysis to check for successful doping. Electron Paramagnetic Resonance (EPR) scans were run on the 1% doped samples to determine the presence of unpaired electrons. Two single crystals were grown with a High Temperature Xenon Floating Zone Furnace.

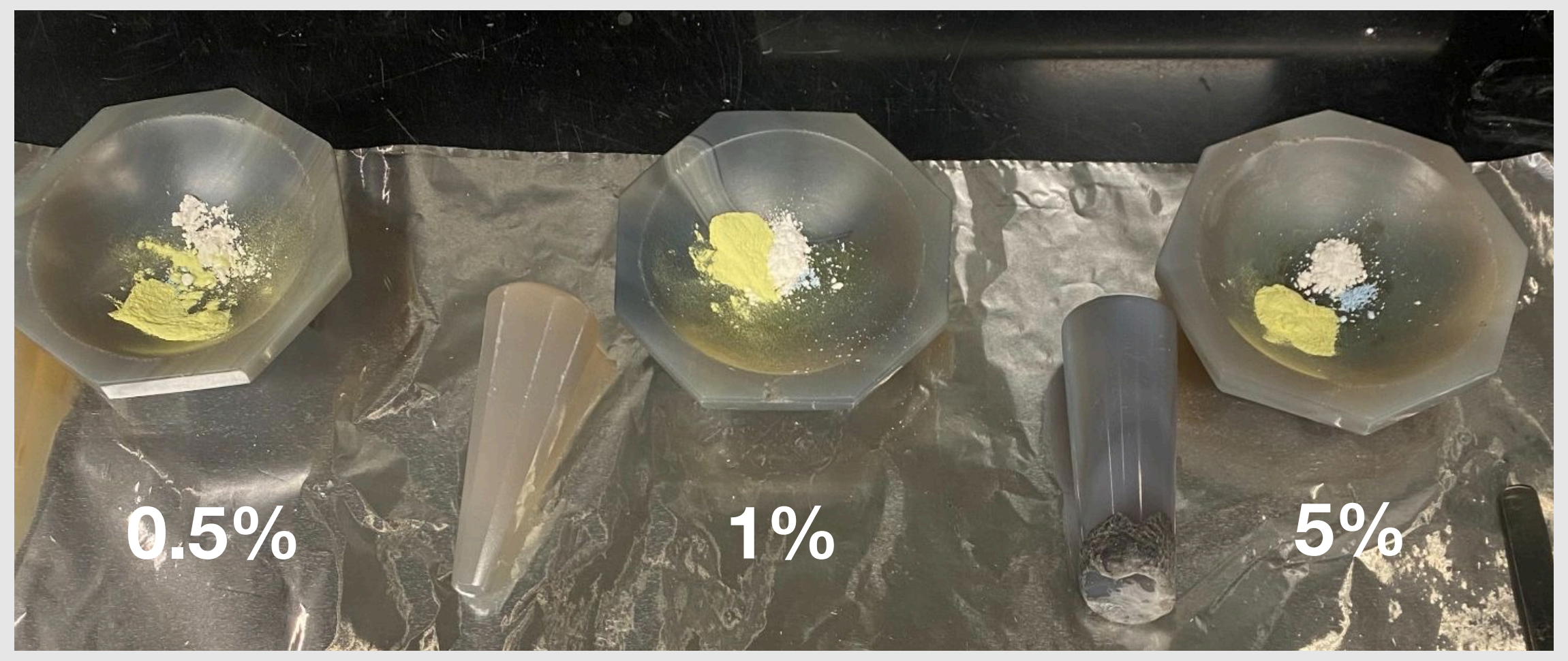

Fig 2. Synthesis process for RE-doped $CaWO_4$

Results

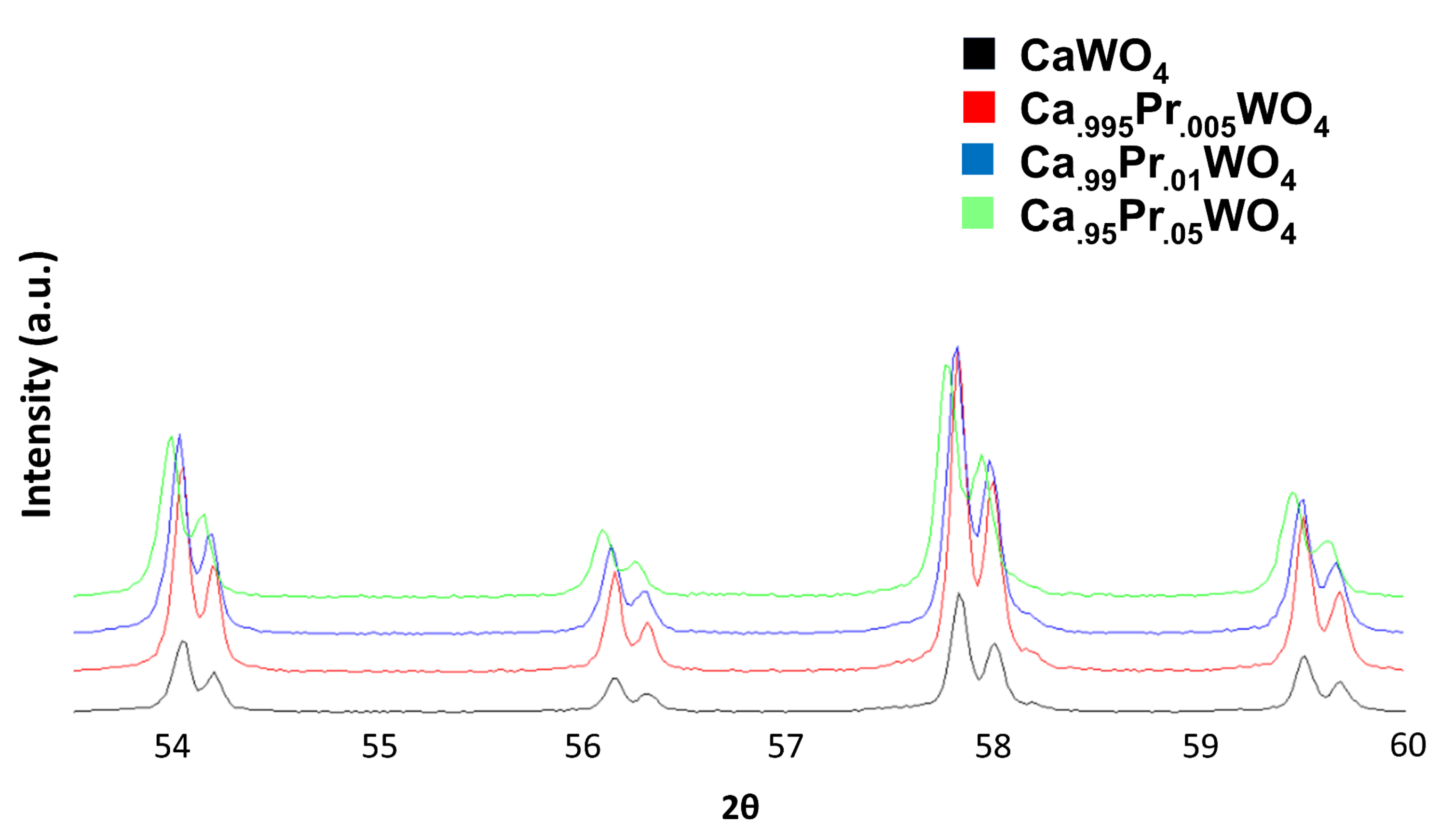

Fig 3. XRD scans of Pr-doped samples and undoped $CaWO_4$

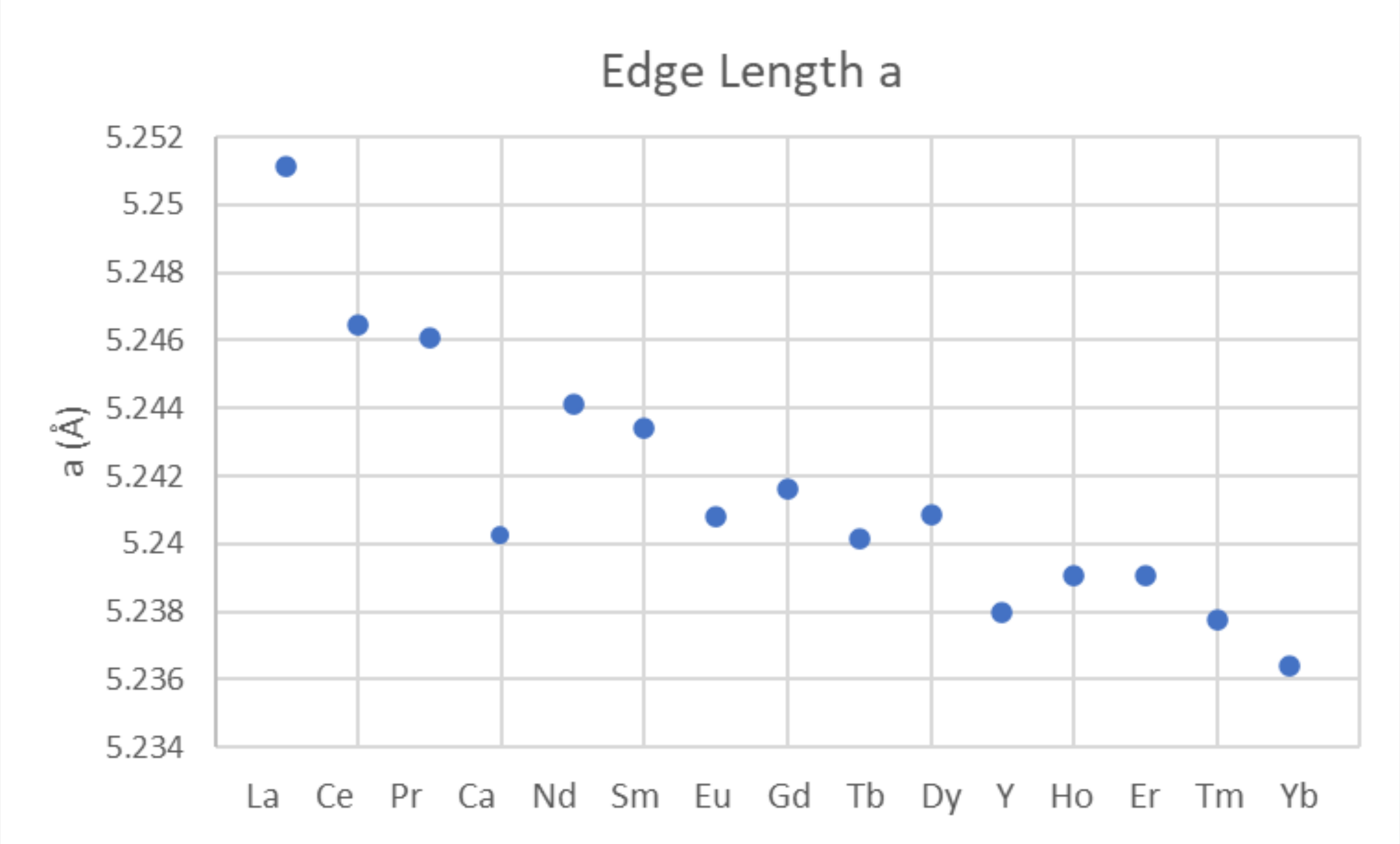

Fig 4. Graph comparing edge length a from Le Bail fit for 5% RE-doped samples

XRD scans comparing the different doping concentrations of a rare earth ion in $CaWO_4$ to undoped $CaWO_4$ revealed a clear peak shift. The peaks shifted to the left for RE ions of a larger atomic radii than calcium and to the right for those of a smaller radii.

Le Bail analysis was used to calculate the edge lengths and volume of the unit cells of the 5% doped samples. The graphs exhibited a roughly linear downward trend in the edge lengths or volume when arranged in order of decreasing RE ion atomic radii. This trend confirmed that the doping was successful.

A distinct sextet of peaks emerged in many of the EPR scans. Unfortunately, these signals were not from any RE-ions but another unpaired electron somewhere in the samples. These peaks were possibly due to tungsten in the form of W^{5+} instead of W^{6+} or some other impurity .

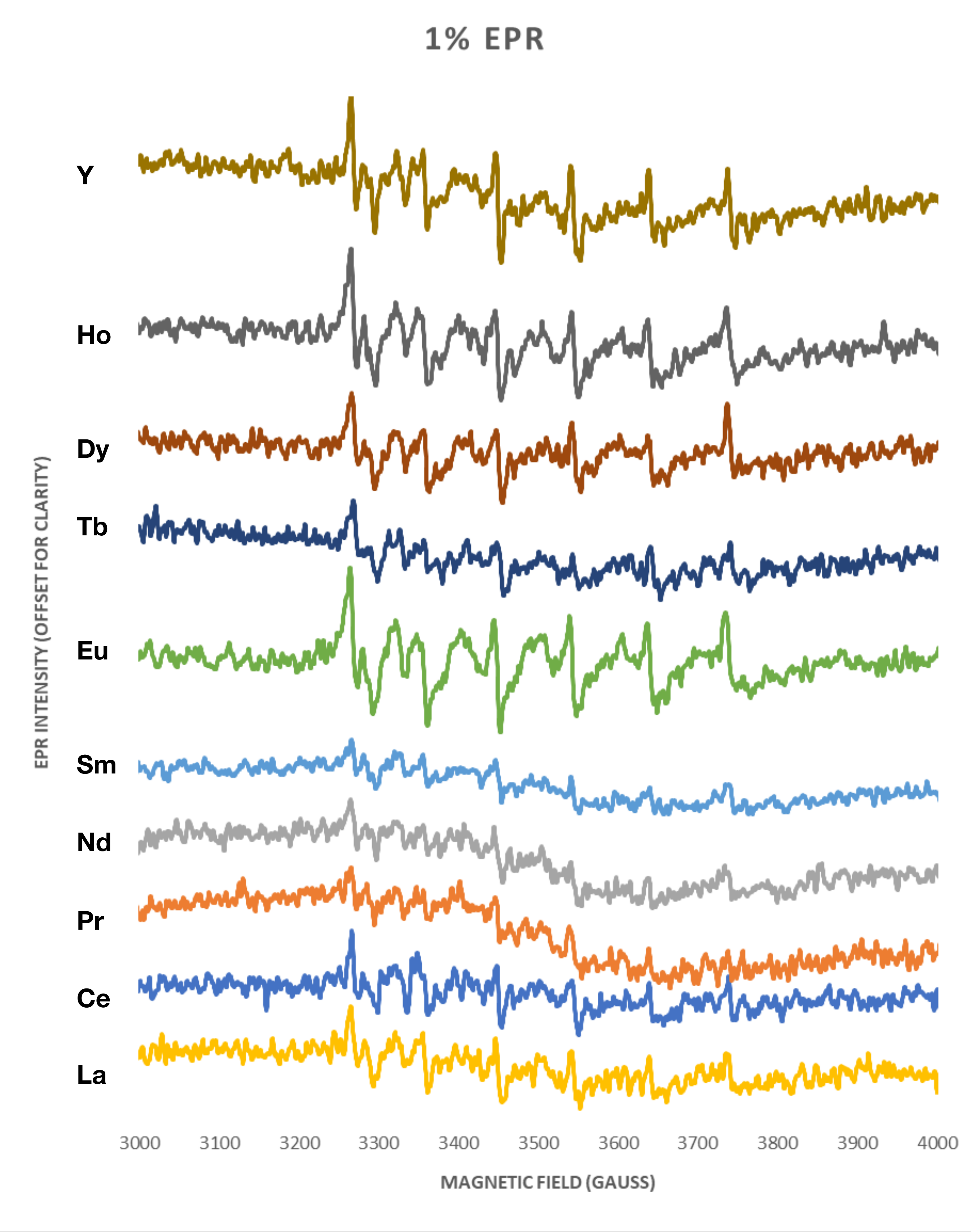

Fig 5. EPR scans from 1% RE-doped samples

Conclusions

The rare-earth ions were successfully doped into the calcium tungstate lattice as demonstrated by Le Bail analysis. For EPR more scans and characterization must be run to determine where the unpaired electrons causing the sextet originated. Optimizing EPR parameters and using an EPR with a stronger magnet may result in clearer signals. To characterize the doped calcium tungstate further, single crystals of each sample should be grown. These growths will assist in revealing which rare-earth ions will perform the best in quantum information processing applications.

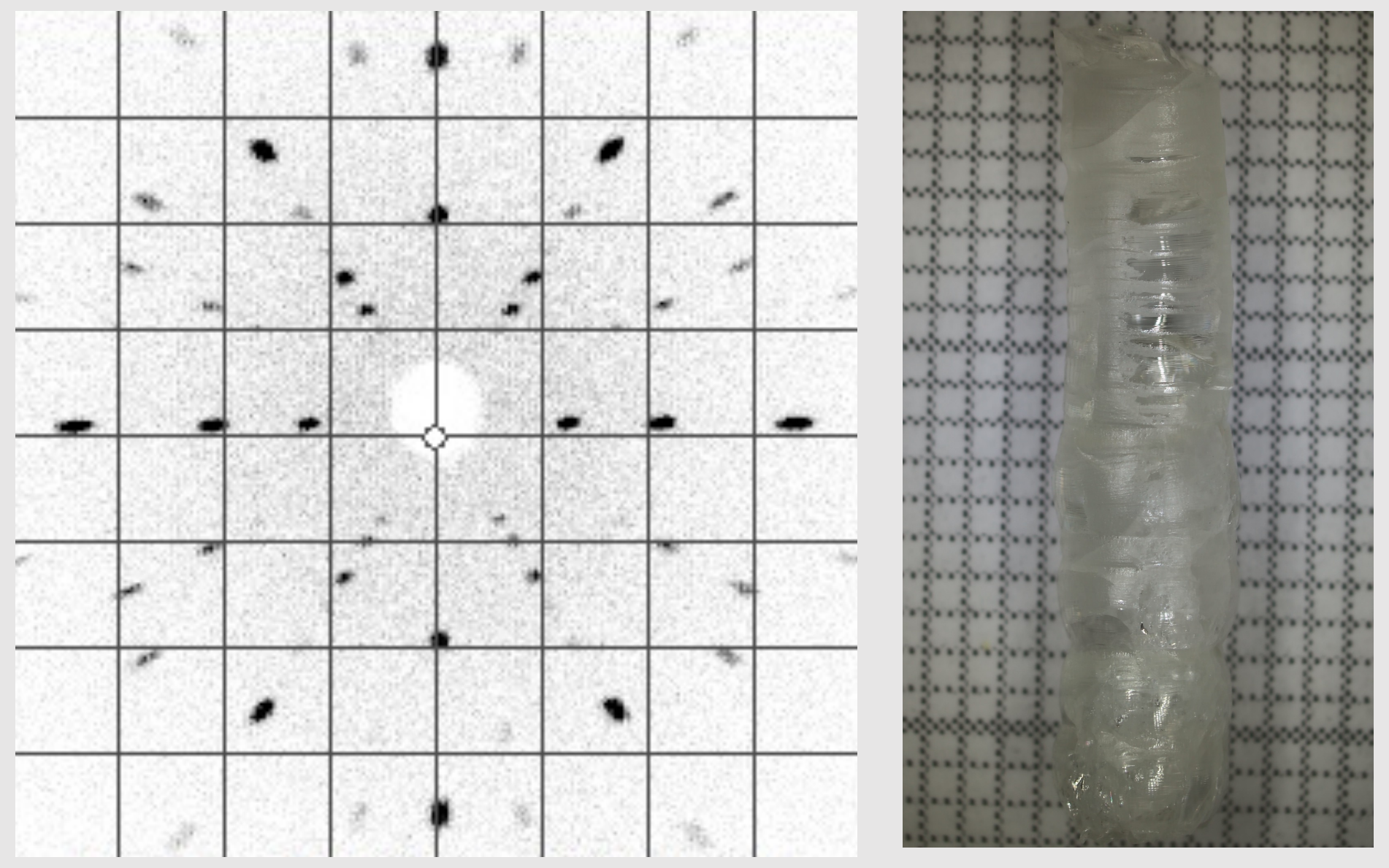

Fig 6 & 7. Laue pattern and image of a $Ca_{1.02}WO_4$ single crystal

Acknowledgements & References

Special thanks to my mentors Satya Kushwaha and Allana Iwanicki for their hands-on support. Thank you to Dr. Tyrel McQueen and Jim Overhiser for inviting me to PARADIM. Lastly, thank you to all the students in the McQueen Lab for all their help.

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3. Abozaid, R. M., et. al. *Science of Sintering* **50**, 446 (2018)

This work was funded by the National Science Foundation (NSF) Platform for the Advanced Realization, Analysis, and Discovery of Interface Materials (PARADIM) under cooperative agreement No. DMR-2039380; **(REU Site: Summer Research Program at PARADIM) under Cooperative Agreement No. DMR-2150446.**