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

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(Dated: August 14, 2023)

Abstract

Qubits made from rare-earth ions such as Er^{3+} are promising candidates for quantum information processing due to their tendency for long spin coherences, stable optical transitions, and potential for quantum transduction[1]. As these ions possess similar chemical characteristics, this project aimed to take a comprehensive look at rare-earth ions doped into $CaWO_4$ to compare their qubit suitability. Multiple concentrations of fifteen rare-earth ions were incorporated into a $CaWO_4$ crystal lattice and analyzed using powder XRD, hyperspectral imaging, and EPR scans. The doping was confirmed to be successful, but the EPR scans exhibited nonideal signals indicating the presence of an unwanted additional unpaired electron. Further characterization of the polycrystalline samples and growths into single crystals are necessary to determine which RE-ions would perform best in quantum information systems.

Introduction

Quantum computing aims to control the two-state nature of quantum bits (qubits) to process data and perform calculations with an efficiency unparalleled by classical computers[2]. Rare-earth (RE) ions doped into a crystal lattice have been found to possess the long spin coherences and sharp optical transitions necessary for quality qubit material[1]. Additionally, Er^{3+} and other RE-ions are being studied for their ability to perform microwave-to-optical transduction which would enable long distance communication between quantum computers[3].

The rare-earth elements are composed of Yttrium, Scandium, and the entire lanthanide series. This project used Yttrium and each lanthanide except Promethium. It was important to identify a highly pure host material that would not negatively influence a qubit's character with a magnetic field or paramagnetic impurities[4]. $CaWO_4$ is a promising choice as both calcium and oxygen are composed almost entirely of nuclear spin-free isotopes[4]. To create the doped material, some of the calcium ions were removed to encourage the RE-ions to fill their sites in the crystal lattice. Once synthesized, the samples could then be analyzed for successful doping, purity, and unpaired electrons with qubit properties.

Methods

The rare-earth doped calcium tungstate was prepared by combining a rare-earth oxide, calcium carbonate, and tungsten trioxide in a mortar and pestle until homogeneous. 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 to 1050°C for twelve hours in a box furnace. Both powder X-ray diffraction (XRD) and hyperspectral imaging were utilized to determine if the RE-ion doping was successful. Each material was reground before being scanned using XRD. The new lattice parameters were calculated by inputting the XRD data into Topaz and running a Le Bail fit. Initially, just the 1% doped samples were scanned under the hyperspectral camera. However, the low doping concentration yielded poor results, so a few of the 5% doped samples were scanned to provide clearer reflectance spectra. Next, Electron Paramagnetic Resonance (EPR) was performed on the 1% doped samples to search for any unpaired electrons. Once characterization of the polycrystalline samples is complete, single crystals of the material should be grown. This can be accomplished using an optical floating zone furnace.

Results and Discussion

A close up of the XRD scans revealed distinct peak shifts to the left or right compared to undoped $CaWO_4$. RE ions of a larger atomic radii than calcium showed increased shifts to the left (as in Fig. 1) as the doping concentration increased; RE-ions of a smaller radii than calcium resulted in rightward peak shifts.

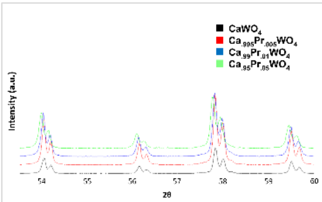

Figure 1. Pr-doped and undoped $CaWO_4$ XRD scans showing leftward peak shift

Le Bail analysis of the XRD data showed the unit cell edge lengths and volumes of the samples decrease roughly linearly when ordered from largest to smallest RE-ion atomic radii as in Fig. 2. This trend in unit cell features indicated the RE-ions were successfully incorporated into the $CaWO_4$ lattice.

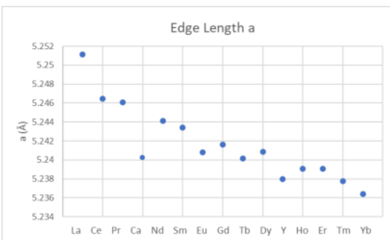

Figure 2. Graph of edge length a from Le Bail fit of the 5% RE-doped samples

The reflectance spectra of some 5% samples were observed by a hyperspectral camera. Their absorbance peaks closely matched those recorded in literature, additionally confirming successful doping.

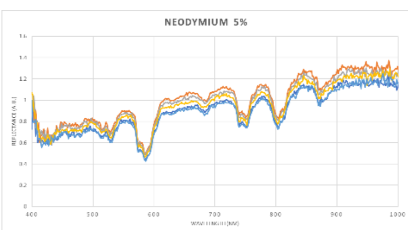

Figure 3. Reflectance spectra of 5% Nd doped sample from hyperspectral imaging

With doping confirmed, EPR scans were run to identify any unpaired electrons present.

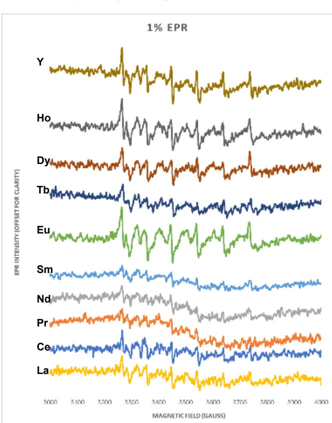

Figure 4. EPR scans of the 5% RE-doped material. No signal was received from Er or Yb

In Fig. 3 a sextet of peaks emerged from many of the EPR scans. While these signals do indicate the presence of unpaired electrons, they do not match signals from the unpaired electrons of RE-ions. This means there is potentially an impurity or defect affecting the samples. A probable explanation is that the sextets originate from tungsten in the form of W^{5+} instead of the expected W^{6+}; however, further characterization must be done to identify the source.

Conclusions

The doping of rare-earth ions into a calcium tungstate host material was accomplished as indicated by Le Bail analysis and hyperspectral imaging. As the EPR scans resulted in nonideal signals, it is not yet possible to determine which RE-ions will perform the best as quantum transducers. Optimizing EPR parameters and using an EPR with a stronger magnet may result in clearer signals. Once the unknown unpaired electron is identified and eliminated, single crystals of the RE-doped material should be grown. This will allow for further characterization and advancement of spin-based qubit materials for quantum information processing.

Acknowledgements

I would like to thank my mentors Dr. Satya Kushwaha and Allana Iwanicki for their support and guidance. Also, thanks to Dr. Tyrel McQueen and the students in the McQueen Lab for all their help this summer. 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.

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