A Study of Tungstate Materials for Use in Quantum Transduction

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Abstract:

The Er^{3+} ion has energetic transitions in the microwave region as well as the optical (infrared) region. Due to these properties, this ion is of interest for use in quantum transduction. Using the chemical formula Ca₁₋ _{2x} $Er_xLi_xWO_4$, different concentrations of Er^{3+} were doped into the CaWO₄ lattice. Single crystals of pure CaWO₄ were grown using a floating zone technique, then using these growth parameters a single crystal of 0.5% Er^{3+} doped CaWO₄ was successfully grown, giving further progress for the possibility of Er^{3+} doped materials for use in transduction.

Introduction

Recently, several companies such as IBM and Google have been investing money in research surrounding the field of quantum computing. With far greater problem-solving capabilities compared to modern computing, quantum computing gives rise to the possibility of new drug and materials discoveries found utilizing the power of this new field of computing. Because the information of these quantum computers is transmitted through microwaves, while the common person receives information transmitted in the optical region (ex. fiberoptic cables), the need for a device which can conduct these conversions becomes apparent.

Transduction is the process of converting electromagnetic radiation of one energy to another energy.¹ In the case of converting a microwave to the optical region, a microwave containing quantum information and an optical photon would enter a transducer, then an optical photon containing quantum information would exit.¹ This energetic transition of interest leads to the need for a material with these energetic transitions. Er³⁺ happens to be an ion which has not only a microwave transition, but an optical transition in the infrared region, causing this ion to be of use for a quantum transducer of the transitions needed in quantum computing.

Since the Er^{3+} ion has an energetic transition of interest for quantum computing, a material with a crystal lattice capable of hosting the Er^{3+} needs to be

used. In past literature, CaWO4 has been found as a suitable lattice host for Er³⁺ ions.² Not only can this material host Er³⁺, but Ca, W, and O are all atoms that have spin neutral isotopes. The possibility for CaWO₄ to be a spin neutral material makes it even more suitable for use in quantum transduction as it would decrease the amount of spin noise in the material which could decrease the coherence of the quantum information transmitted through a quantum computer. With such advantages CaWO₄ demands the development of clean samples, which utilizing an optical floating zone is a well-accepted method to do so. Thus, the goal of this project was to first grow single crystals of CaWO₄ using the floating zone method, then synthesize CaWO₄ doped with varying concentrations of Er³⁺ ions and grow a single crystal of an Er³⁺ doped system.

Methods and Discussion

CaWO₄ was synthesized by combining equal molar amounts of CaCO₃ and WO₃. This mixture was put in a crucible and put in a box furnace. From room temperature, a ramp rate of 100°C/hr was used until 1,000°C was achieved. The furnace remained at this temperature for 24 hrs, then using the same ramp rate returned to room temperature. Powder X-ray diffraction (XRD) was then used to characterize pure CaWO₄. The pure CaWO₄ was then made into rods, which were sintered at 1,400°C for 24 hrs.

Pure rods of CaWO₄ were then placed in the High-Pressure Floating Zone furnace at the PARADIM Bulk Crystal Growth facility at JHU. To initially melt the rods, the aperture of the Xenon lamp was opened by 19%. Upon joining the molten zone, the rods were translated downwards at a rate of 2 mm/hr, while counter rotating at a rate of 10 rpm. Although the ideal growth conditions seemed to be met, the Xenon lamp aperture had to be monitored and increasingly opened to ensure molten zone stability. Two growths of CaWO₄ were performed, both demonstrating crystallinity through Laue XRD. However, the second growth contained an apparent transparent portion of crystal, without the presence of separate grains showing success for the single crystal growth of CaWO₄.



Figure 1. Single crystal of CaWO₄ and Laue XRD

To synthesize Er³⁺ doped CaWO₄, CaCO₃, WO₃, Er₂O₃ and Li₂CO₃ were combined to achieve a molecular equation of Ca_{1-2x}Er_xLi_xWO₄. The presence of the Li⁺ is to provide charge neutrality, the presence of charges in the lattice is another form of noise which can decrease coherence of quantum information. Mixtures of the components were combined and then pressed into approximately 1.0 g pellets, then put into a box furnace with the same heating program as the CaWO₄ synthesis. When the pellets were removed from the furnace, they appeared to have a clear visual trend demonstrating an increase of Er³⁺ doping as an increase in the pink color of the samples. The lowest doping concentrations, 0.1% and 0.5%, appeared white while the highest doping concentration, 10%, appeared bright pink. This increase in Er³⁺ doping was further confirmed through the use of hyperspectral imaging. CaWO₄ with no doping showed no peaks, making sense due to the white color of the powder. However, as Er³⁺ doping increased, absorbance peaks at 525 nm and 650 nm appeared and increased in intensity demonstrating the integration of the Er³⁺ in the lattice. This is further demonstrated through powder XRD, in which the peaks have a clear shift towards higher angles as the concentration of Er³⁺ increases. Thus, the Er³⁺ doped CaWO₄ was able to be successfully synthesized.



Figure 2. Powder XRD pattern of various Er^{3+} concentrations doped in CaWO₄

A bulk sample of 0.5% Er³⁺ doped CaWO₄ was synthesized the same way previously mentioned for CaWO₄. This bulk sample was then made into rods for use in the High-Pressure Floating Zone furnace and then a single crystal growth was performed of the Er³⁺ doped sample using the same growth parameters as the CaWO₄ growth. This single crystal demonstrated some transparency in different locations; however, the molten zone was somewhat unstable and the parameters had to be monitored closely. Also, this crystal cracked near the base of the growth likely from thermal shock within the furnace. When removed from the furnace, the crystal broke apart in several places but utilizing Laue XRD, crystallinity was still present to a degree.



Figure 3. Single crystal of $Ca_{0.99}Er_{0.005}Li_{0.005}WO_4$ and Laue XRD

Conclusions

Although no completely pure $CaWO_4$ crystal was made, those that were demonstrated high amounts of crystallinity showing that this was a promising start towards the synthesis of single crystals for this material via optical floating zone technique. Part of the reason cracks may be appearing in the single crystal is due to thermal shock, which could be mitigated in future experiments with the presence of another heating element within the furnace below the hot zone.

Several samples of Er³⁺ doped CaWO₄ were also synthesized with differing concentrations of dopant. The integration of dopant was demonstrated through hyperspectral imaging, powder XRD, and plotting of lattice parameters. Also, a sample of low Er³⁺ doping was able to be grown as a single crystal using a floating zone furnace. This low amount of doping would be ideal for quantum transduction, but further characterization needs to be done using EPR to look at the energetic transitions of the material. However, this project demonstrated an overall success in the first steps towards the synthesis of a material for use in quantum transduction.

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