Synthesis and Characterization of Multi-Purpose Functional Transport Materials

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Primary PARADIM Tools Used: Laser diode floating zone, Spark plasma sintering instrument

Abstract:

Understanding the intricacies of electronic phenomena in new functional transport materials will give greater insight into fundamental understandings and applications of materials. The materials investigated have interesting properties leading to applications in quantum computing in the case of topological Kondo Insulator candidate YbB_{12} and waste heat recovery for the new thermoelectric $Cu_2GeZnTe_4$. Previous reports have shown YbB_{12} as having quantum properties, but with the synthesis of this compound being difficult, these quantum phenomena could possibly be attributed to material defects rather than the intrinsic properties of the YbB_{12}. By using PARADIM's laser diode floating zone furnace to grow single crystals of the Kondo Insulator, the instrument allows for a well-defined heating profile for a higher quality synthesis. The quality of the material can be assessed through X-ray diffraction and Laue measurements, and the materials quantum properties tested through various electronic and magnetic property measurements. The desired chemical composition of $Cu_2GeZnTe_4$ was determined using a database called TE Design Lab, which consists of theoretical and experimental data of potential quality thermoelectric materials gathered by Dr. Eric Toberer. Because of the low temperature barrier for synthesizing the isostructural compound to the Cu_2-II-IV-VI_4 family of thermoelectrics, the $Cu_2GeZnTe_4$ is synthesized and densified using spark plasma sintering to further determine its thermal and electrical conductivity.

Summary of Research:

Ytterbium dodecaboride (YbB_{12}) rods were made by pressurizing Yb_2O_3 and B powder in stoichiometric proportions in accordance to the reaction $Yb_2O_3 + 27B \rightarrow 2YbB_{12} + \uparrow 3BO$. The rods were pressurized through vacuum, hydrostatic press and sintered using xenon lamps. Feed and seed rods were then set up with a molar equivalent of a YbB_{30} pellet on top of the seed rod to stabilize the growth for the floating zone crystal growth. The top of the seed rod is then melted, the two rods are connected and slowly moved through the floating zone in order to grow a single crystal, which is verified through powder X-ray diffraction, single crystal X-ray diffraction and Laue measurements. To determine the quality of the crystal, preliminary measurements, like heat capacity, were conducted for comparison to literature values.

To prepare the thermoelectric material $Cu_2GeZnTe_4$, the ternary Cu_2GeTe_3 and the binary ZnTe we synthesized from retrospective metal elements and melted in a vacuum sealed in a glass quartz tube, with the ternary in a boron nitride crucible. The purity of the ternary and binary were confirmed with powder X-ray diffraction, then the two compounds were ground together in stoichiometric proportions and put into a graphite crucible to put into a spark plasma sintering instrument in order to synthesize and densify the compound for resistivity measurements.

The purity of the compound was confirmed from powder X-ray diffraction, which confirmed reactions up to 90% completion.

Results and Conclusions:

A single crystal of YbB_{12} was confirmed as a pure, single crystal of the compound and the heat capacity measurements proved to be similar to literature measurements, with a slight peak at around 4 K from the presence of helium. The powder X-ray diffraction pattern of $Cu_2ZnGeTe_4$ confirmed that the reaction progressed to 90% by weight, leaving room for improvement in this synthesis.

Future Work:

Future work for the Kondo Insulator YbB_{12} includes various structural, electronic and magnetic measurements on each lattice surface in order to determine the presence of a magnetic surface state or the creation of an insulative state from the hybridization of d and f orbitals, and to determine which surface these state's potentially exist in.

Future work for the thermoelectric material $Cu_2ZnGeTe_4$ includes perfecting the synthesis of the compound and then measuring structural and electronic properties through measurements like heat capacity, resistivity and thermal conductivity.

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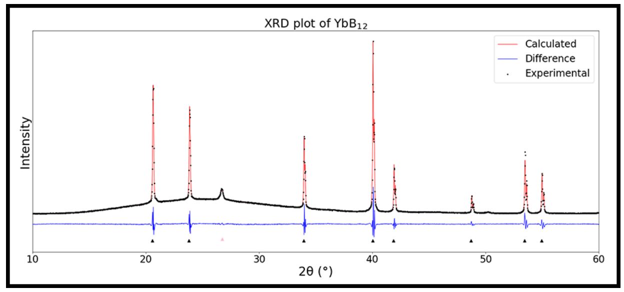

Figure 1: Powder X-ray diffraction of single crystal YbB_{12}, demonstrating the purity of the sample. The peak at around 26 2θ. (°) represented by the pink marker is from the glass slide the sample rested on.

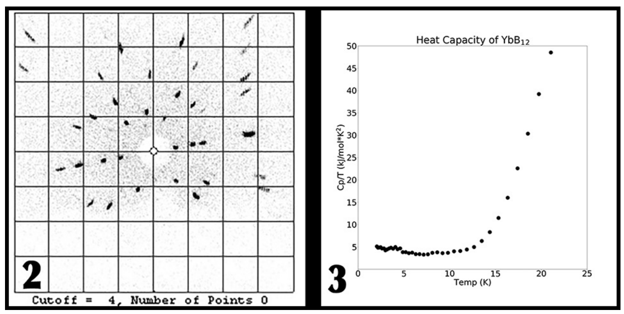

***Figure 2, left:** Laue single crystal measurements that determine the lattice plane in the crystal. **Figure 3, right:** Heat capacity of single crystal YbB_{12} from 0 K to 25 K.*

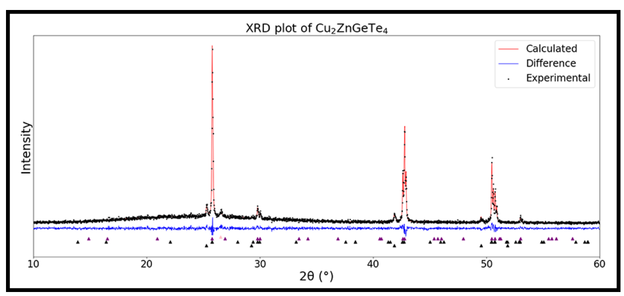

Figure 4: Powder X-ray diffraction of $Cu_2ZnGeTe_4$, showing the reactions progression, where the purple markers denote the quaternary, the black markers denote the ternary and binary, and the pink marker denoting a trace amount of graphite in the sample.