Exploring Thermoelectric Properties of Thin Film YbB$_x$

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Introduction:

Thermoelectric materials have the potential as sources of renewable energy because they can generate electricity from heat with no waste, and vice versa, by the Peltier and Seebeck effects. To be a good candidate for thermoelectric power generation, a material must have a high electrical conductivity σ, high Seebeck coefficient S, and low thermal conductivity κ, in order to maximize the figure of merit, ZT, which is related to a materials power conversion efficiency. The ZT value is given by the equation:

$$ZT = \frac{(S^2\sigma)T}{\kappa}$$

Typical commercial thermoelectrics have a ZT $\approx$ 1, but the necessary ZT for a good power conversion efficiency depends on the type of application [1].

Certain metal-boride compounds, such as SrB$_6$, have been known to make good thermoelectrics [2], as have bulk ytterbium-boride compounds [3,4]. Previously, only bulk YbB$_6$ has been investigated for its thermoelectric properties. Our research focuses instead on thin film ytterbium borides of many different stoichiometries. Thin film thermo-electrics are important to study because of their niche applications, such as use in microsensors or on flexible substrates [5].

Measurements and Results:

X-Ray Diffraction. X-ray diffraction (XRD) was used in order to determine the chemical composition of our thin films. The XRD data were collected over a 2θ range of 10-110°, at a rate of 2.0-2.8°/min, with a 0.02°/step. We first performed XRD analysis on our sapphire substrate in order to exclude the reflections originating from the substrate. Since the penetration depth of the x-rays were much larger than the thickness of our films, reflections with the highest intensities (and corresponding angle) were assigned to the substrate, and the remaining peaks correspond to reflections from the sample. Our deposition process produced highly orientated films, which resulted in XRD peaks of different intensities than those of a powder sample. The two primary YbB$_x$ stoichiometries we observed from XRD analysis in our films were either YbB$_6$ or YbB$_2$, as shown in Figures 2 and 3. These two compounds differ greatly in their crystal structure: YbB$_6$ has a cubic structure with space group Pm-3m and a lattice constant of 4.1444 Å, while YbB$_2$ has a hexagonal structure with space group P6/mmm and a lattice constant of with lattice parameters 3.2503 Å × 3.2503 Å × 3.7215 Å [6].

Our XRD measurements did not allow us to deduce the exact stoichiometry of our films, and both our XRD data and the large variances in our measurements of electrical conductivity and Seebeck coefficient suggest that some of our samples may be non-stoichiometric.

Electrical Properties Measurements. The Ulvac ZEM-3 was used to measure the electrical properties of our thin films, using a 4-point probe method to measure the electrical resistivity and the Seebeck coefficient of our films simultaneously. We chose a temperature range of 325-575 K to measure these properties, as we could not go any higher without possibly damaging the electrical contacts. Measurements were performed several times on the same sample, in different locations on the sample in order to test for good uniformity. The color legend for all measured samples is provided in Figure 4.
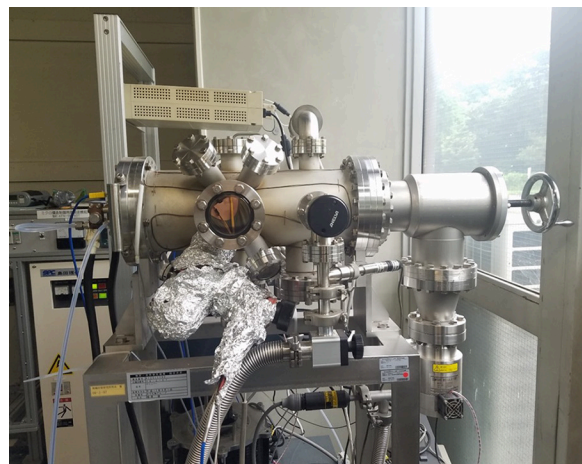

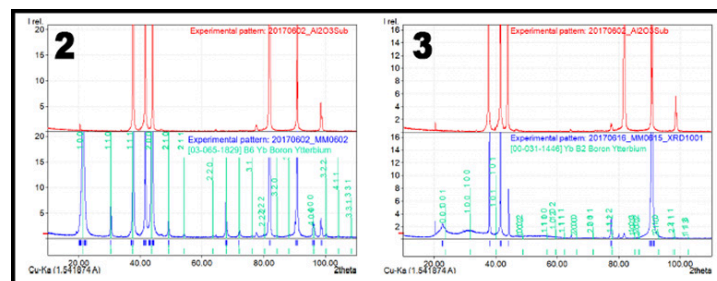*Figure 1: An image of our custom-built CVD tool.*

Figure 2, left: XRD analysis of a YbB$_6$ film. Figure 3, right: XRD analysis of a YbB$_2$ film.

As seen in Figure 5, our results from the Seebeck coefficient measurements show that our films all present n-type semi-conducting behavior. Together, these results suggest that our films may all be degenerate semiconductors.

Our results from the resistivity measurements were not always very consistent for one given sample, and we can see from Figure 6 different slopes for different measurements on the same sample. However, these measurements remain within the same order of magnitude. Moreover, across measurements from different samples, the differences between individual measurements from each given sample are negligible, as can be seen from Figure 7.

The power factor, calculated from the Seebeck coefficient and the resistivity, gives us a clear understanding of which films might perform the best as thermoelectrics. For thermal properties measurements, we chose the best YbB_6 and the best YbB_2 film in order to proceed with measurements.

Time-Domain Thermoreflectance. We measured the thermal diffusivity of our thin films, necessary for calculating the thermal conductivity, using a picosecond time-domain thermoreflectance method [7]. After depositing an aluminum thin film on our sample, a picosecond laser was used to heat the sample, and a probe laser was used to measure how the reflectivity changed with the changing temperature of the sample. This process is shown in Figure 9. By fitting the curve of thermoreflectance vs. time, we calculated the thermal diffusivity of our thin films at room temperature.

Results and Conclusions:

From the thermal diffusivity measurements we were able to calculate room temperature thermal conductivity values for two of our samples. Using the power factor values at $T \approx 562$ K, we calculated ZT values for these two films (Note: we expect the thermal conductivity to decrease with higher temperature, so the ZT at this temperature should be a slight overestimate). As shown in Table 1, we see that the ZT value for this YbB_6 sample to be an order of magnitude better than that of the YbB_2 sample. Our results suggest that thin film YbB_6 may make a better thermoelectric than thin film YbB_2 because of its higher ZT value. However, future work remains to be done on this research, such as finding the thermal conductivity at higher temperatures for more films, and potentially also examining thin film YbB_4 as a viable thermoelectric.

Acknowledgements:

References:

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[5]   H. Baltes, et al. Sensors Set, 2008, pgs. 13-55.

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[7]   Y.K. Koh, et al. J of Applied Physics 105, 054303 (2009).

Figure 4: The color legend for all the electrical properties measurements.
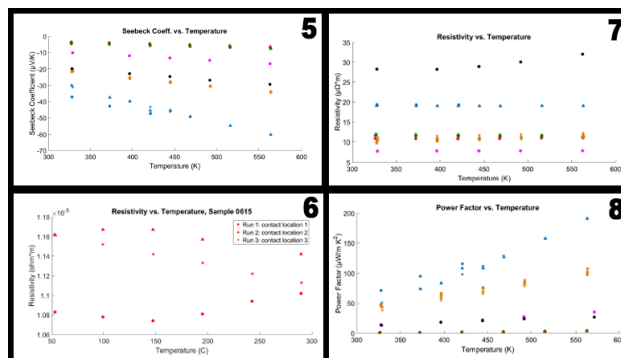

Figure 5: The Seebeck coefficient measurements over a range of temperatures for different thin films. Figure 6: The resistivity measurements over a range of temperatures for the same thin film. Figure 7: The resistivity measurements over a range of temperatures for different thin films. Figure 8: The power factor, calculated from the Seebeck coefficient and resistivity measurements, over a range of temperatures for different thin films.
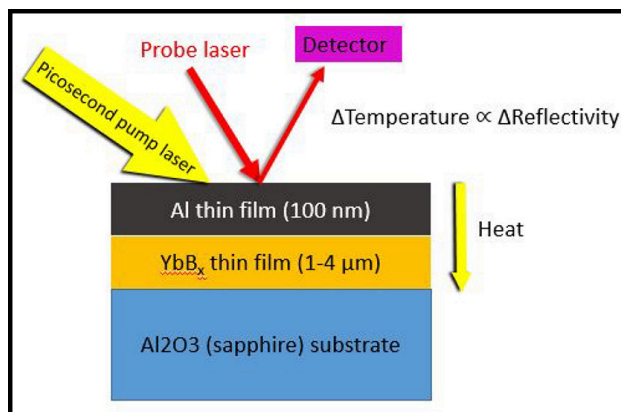

Figure 9: The process by which time-domain thermoreflectance works.

$T \approx 562$ K	YbB_6	YbB_2
Power Factor (μ W/ mK)	191	4
Room Temp Thermal Cond. (W/mK)	2.540	1.064
ZT	≈ 0.04	$\approx 2 \times 10^{-3}$

Table 1: The table of power factor at $T \approx 562$ K, room temperature thermal conductivity, and calculated ZT from one YbB_6 (blue sample in Figure 4) and one YbB_2 sample (red sample in Figure 4).

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