

High Temperature Grain Boundary Resistance in $\text{Yb}_{14}(\text{Mg},\text{Mn})\text{Sb}_{11}$ Thermoelectrics

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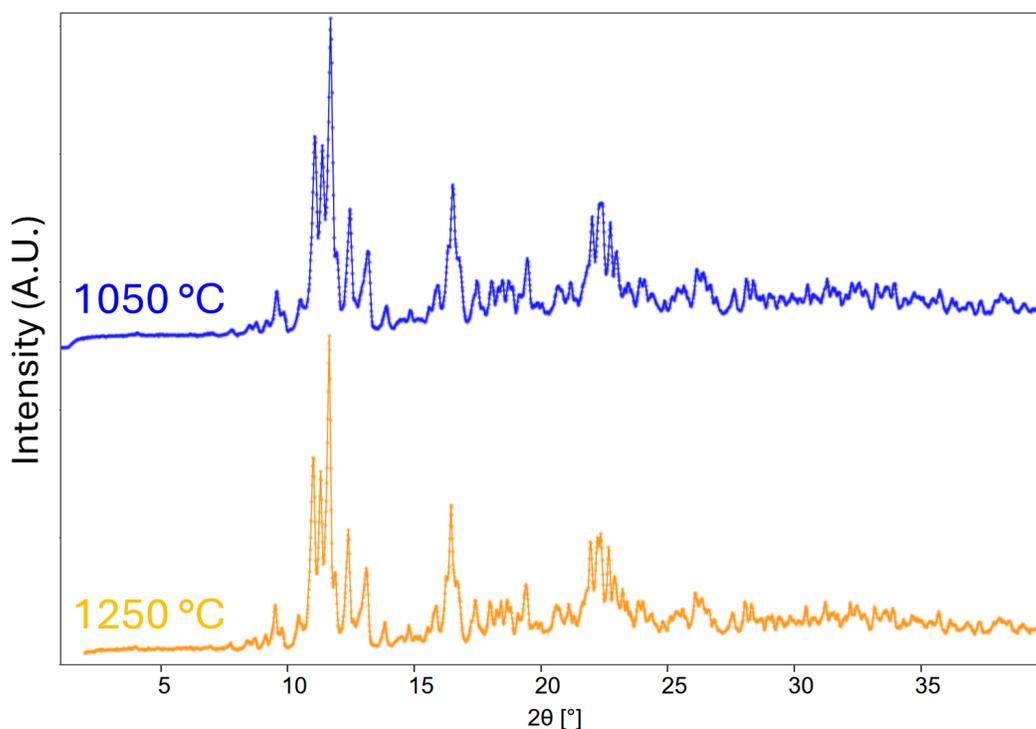
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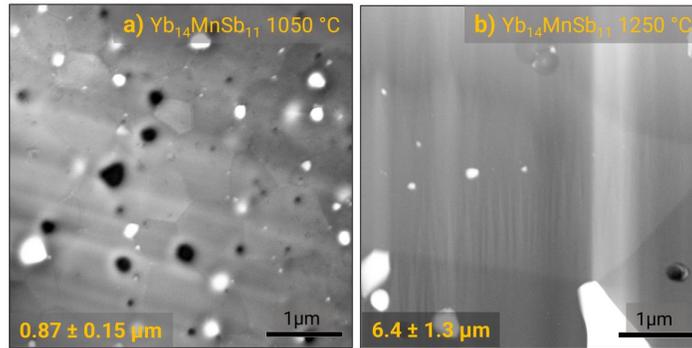
S1: Additional X-Ray Diffraction of the 1050 °C and 1250 °C Samples



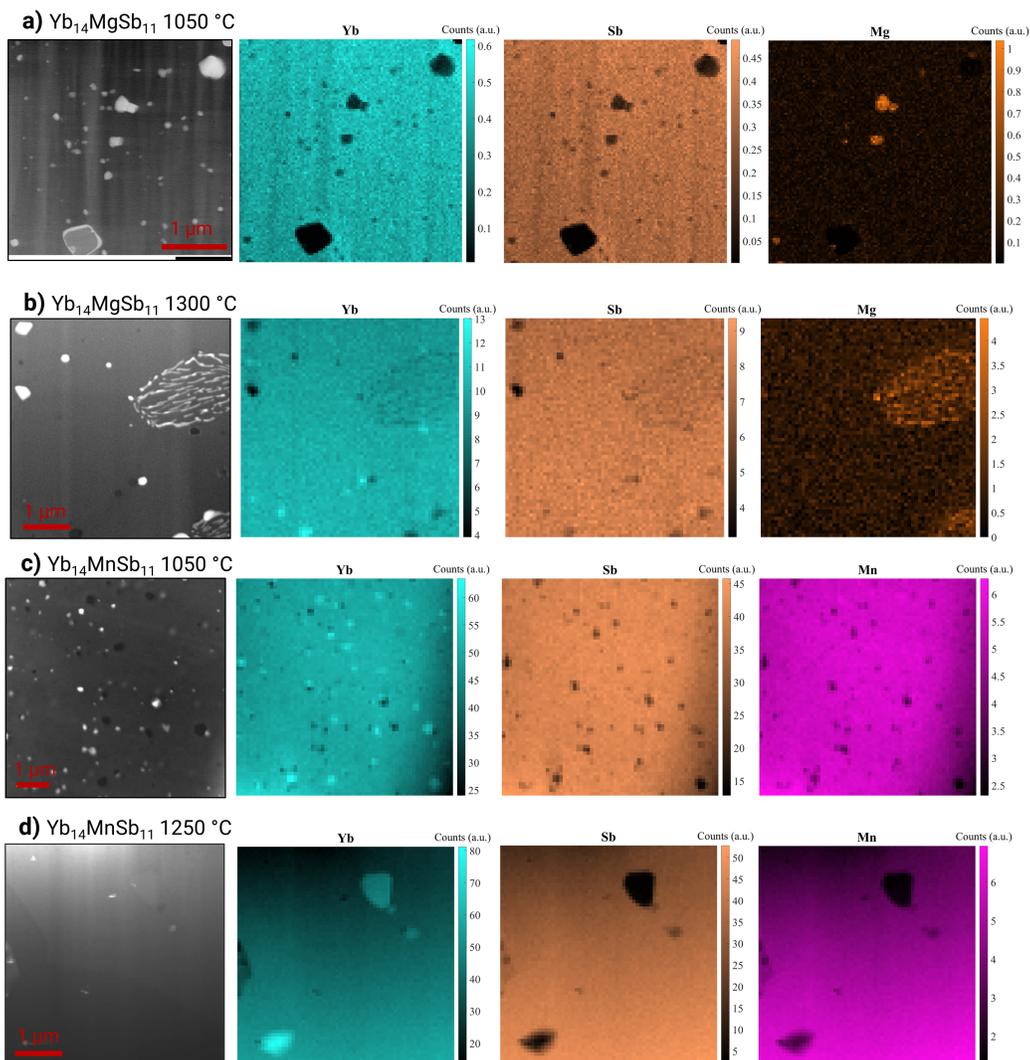
S2: Grain Size Measurement Details

| sample | Mean Intercept Length Method | | | | | sample | Mean Intercept Length Method | | | | |
|---|------------------------------|------------------|--------|----------------------------|--|--|------------------------------|------------------|--------|------------------------------|------------------------------|
| | Line | Line Length (μm) | Counts | mean intercept length (μm) | Grain Size (μm) | | Line | Line Length (μm) | Counts | mean intercept length (μm) | Grain Size (μm) |
| Yb ₁₄ MnSb ₁₁ 1050 C | 1 | 3.368 | 6 | 0.5614 | 0.842 | Yb ₁₄ MgSb ₁₁ 1050 C | 1 | 4.491 | 9 | 0.4990 | 0.749 |
| | 2 | 3.368 | 5 | 0.6737 | 1.011 | | 2 | 4.491 | 9 | 0.4990 | 0.749 |
| | 3 | 3.368 | 5 | 0.6737 | 1.011 | | 3 | 4.491 | 10 | 0.4491 | 0.674 |
| | 4 | 3.380 | 7 | 0.4828 | 0.724 | | 4 | 4.491 | 12 | 0.3743 | 0.561 |
| | 5 | 3.380 | 5 | 0.6759 | 1.014 | | 5 | 4.491 | 10 | 0.4491 | 0.674 |
| | 6 | 3.380 | 8 | 0.4224 | 0.634 | | 6 | 4.491 | 10 | 0.4491 | 0.674 |
| | Average sdt | | | | 0.872 0.152 | | Average sdt | | | | 0.680 0.063 |
| Yb ₁₄ MnSb ₁₁ 1250 C | 1 | 10.896 | 2 | 5.4480 | 8.172 | Yb ₁₄ MgSb ₁₁ 1250 C | 1 | 6.892 | 9 | 0.7658 | 1.149 |
| | 2 | 10.896 | 3 | 3.6320 | 5.448 | | 2 | 6.892 | 5 | 1.3784 | 2.068 |
| | 3 | 10.896 | 3 | 3.6320 | 5.448 | | 3 | 6.892 | 5 | 1.3784 | 2.068 |
| | 4 | 10.896 | 2 | 5.4480 | 8.172 | | 4 | 20.340 | 18 | 1.1300 | 1.695 |
| | 5 | 10.896 | 3 | 3.6320 | 5.448 | | 5 | 13.534 | 14 | 0.9667 | 1.450 |
| | 6 | 10.896 | 3 | 3.6320 | 5.448 | | 6 | 6.767 | 8 | 0.8459 | 1.269 |
| | Average sdt | | | | 6.356 1.284 | | Average sdt | | | | 1.616 0.361 |
| | | | | | Yb ₁₄ MgSb ₁₁ 1300 C | 1 | 10.427 | 5 | 2.0854 | 3.128 | |
| | | | | | | 2 | 10.427 | 5 | 2.0854 | 3.128 | |
| | | | | | | 3 | 10.427 | 3 | 3.4757 | 5.214 | |
| | | | | | | 4 | 10.427 | 3 | 3.4757 | 5.214 | |
| | | | | | | 5 | 10.427 | 7 | 1.4896 | 2.234 | |
| | | | | | | 6 | 10.427 | 8 | 1.3034 | 1.955 | |
| | | | | | | Average sdt | | | | 3.479 1.300 | |

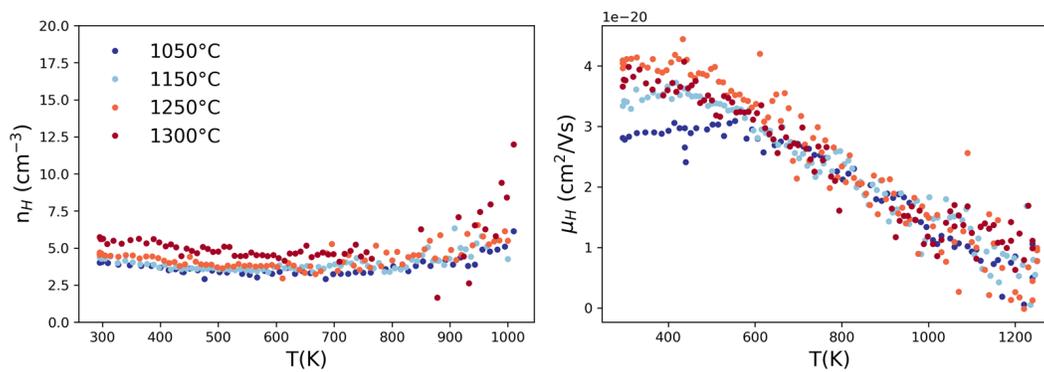
S3: Yb₁₄MnSb₁₁ Grain Size



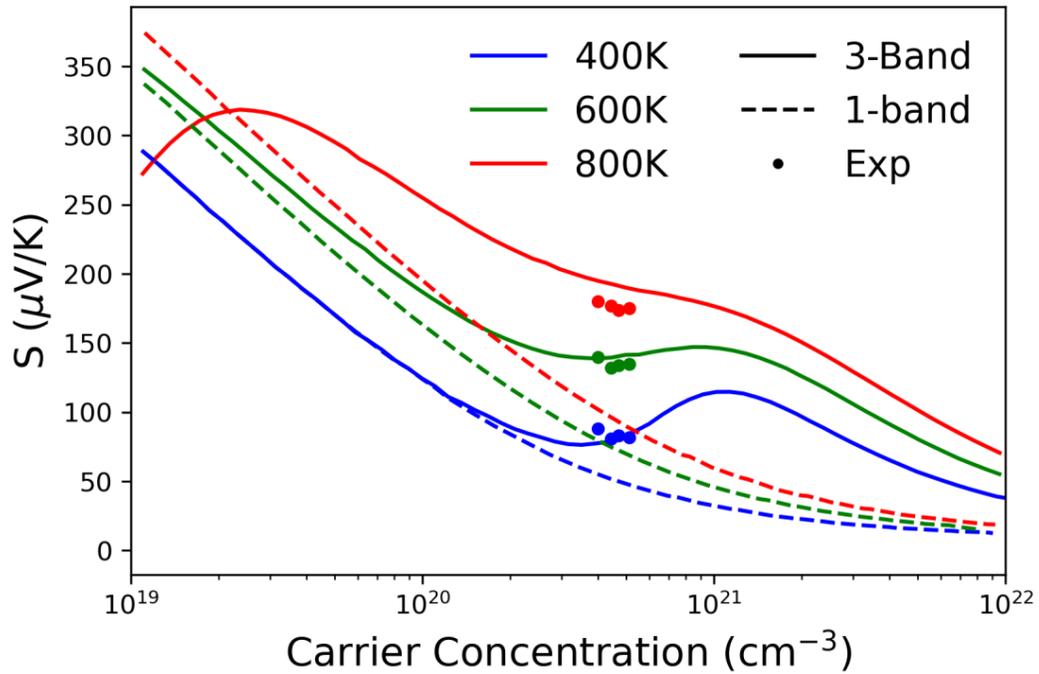
S4: Energy Dispersive X-Ray Spectroscopy



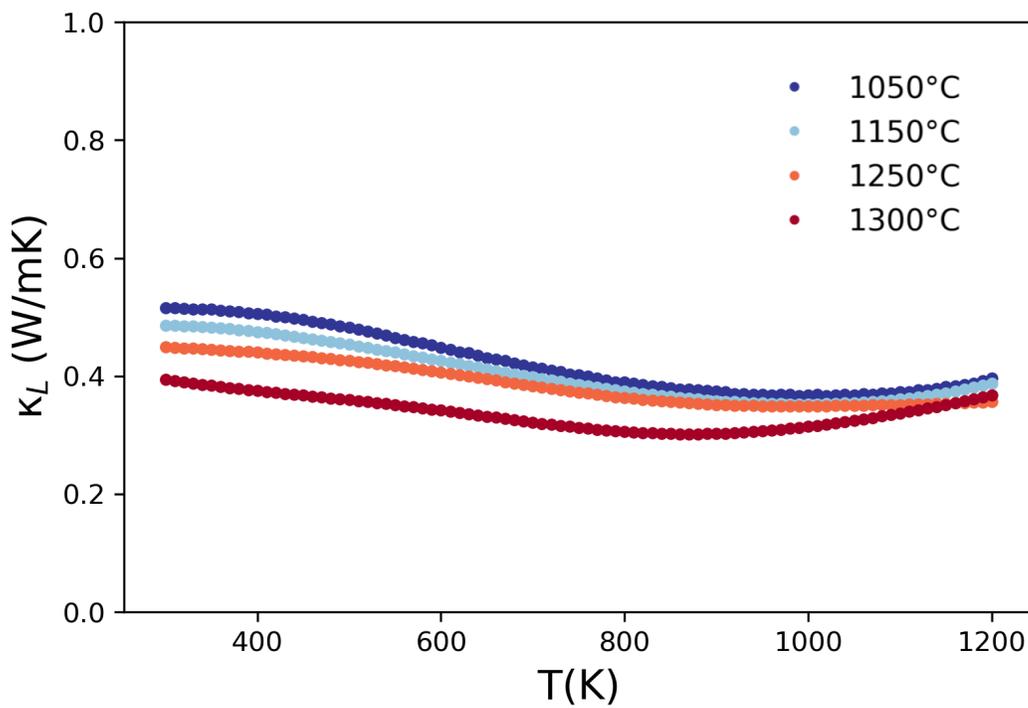
S5: Hall Carrier Concentration and Mobility in $\text{Yb}_{14}\text{MgSb}_{11}$



S6: Single and Multiband Pisarenko Plots for $\text{Yb}_{14}\text{MgSb}_{11}$

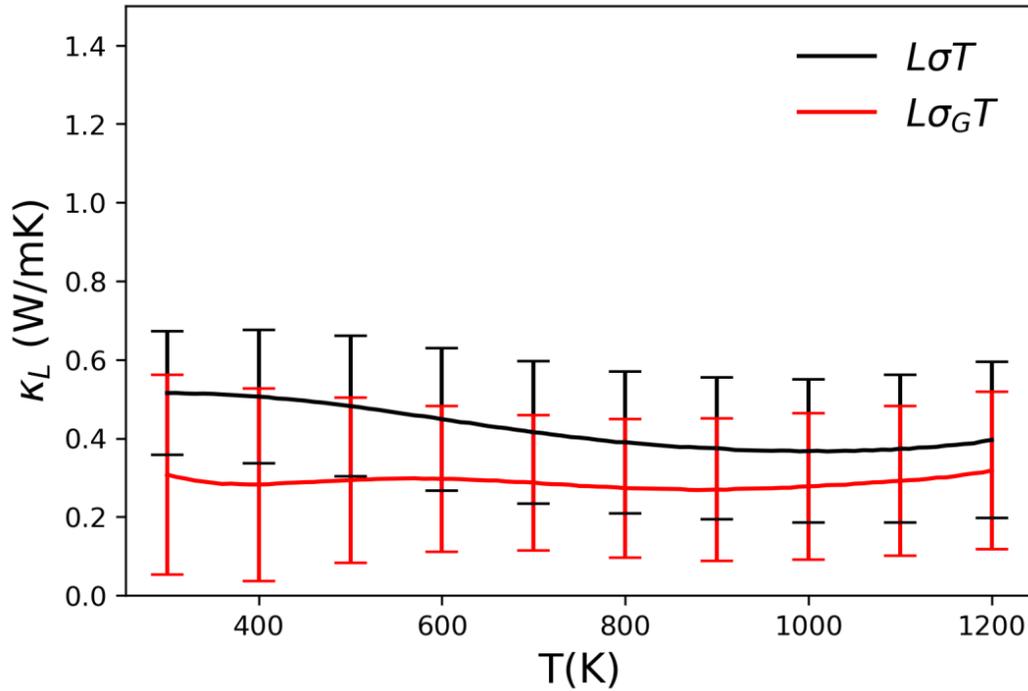


S7: Lattice Thermal Conductivity calculated with standard Wiedemann Franz Law



S8: Uncertainty in lattice thermal conductivity measurements

The error bars for κ_L were calculated using an uncertainty of 5% in Lorenz number,¹ 5% in electrical conductivity,² and 10% in measured thermal conductivity.³ The uncertainty in the grain conductivity was calculated by taking the standard deviation in the x intercept in the ρ versus $1/d$ line from Equation 2 and Figure 7.



References

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3. Heremans, J. P. & Martin, J. Thermoelectric measurements. *Nat. Mater.* **23**, 18–19 (2024).