Thermoelectric Properties of $CuBi_xSb_{1-x}Te_2$ Bulk Alloys

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RTNN

AIF analytical instrumentation facility

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CuBiSbTe2 Material System

- Why is this material system interesting?
  - Unusually low thermal conductivities in preliminary measurements
  - Potentially significant ZTs prior to processing steps such as annealing and/or microwaving
  - Even amorphous samples (melt-quenched without any spark plasma sintering) show ultra-low thermal conductivity
  - Potentially useful in waste heat recovery devices, among other applications of thermoelectrics

ZT

TE Power

Electrical Conductivity

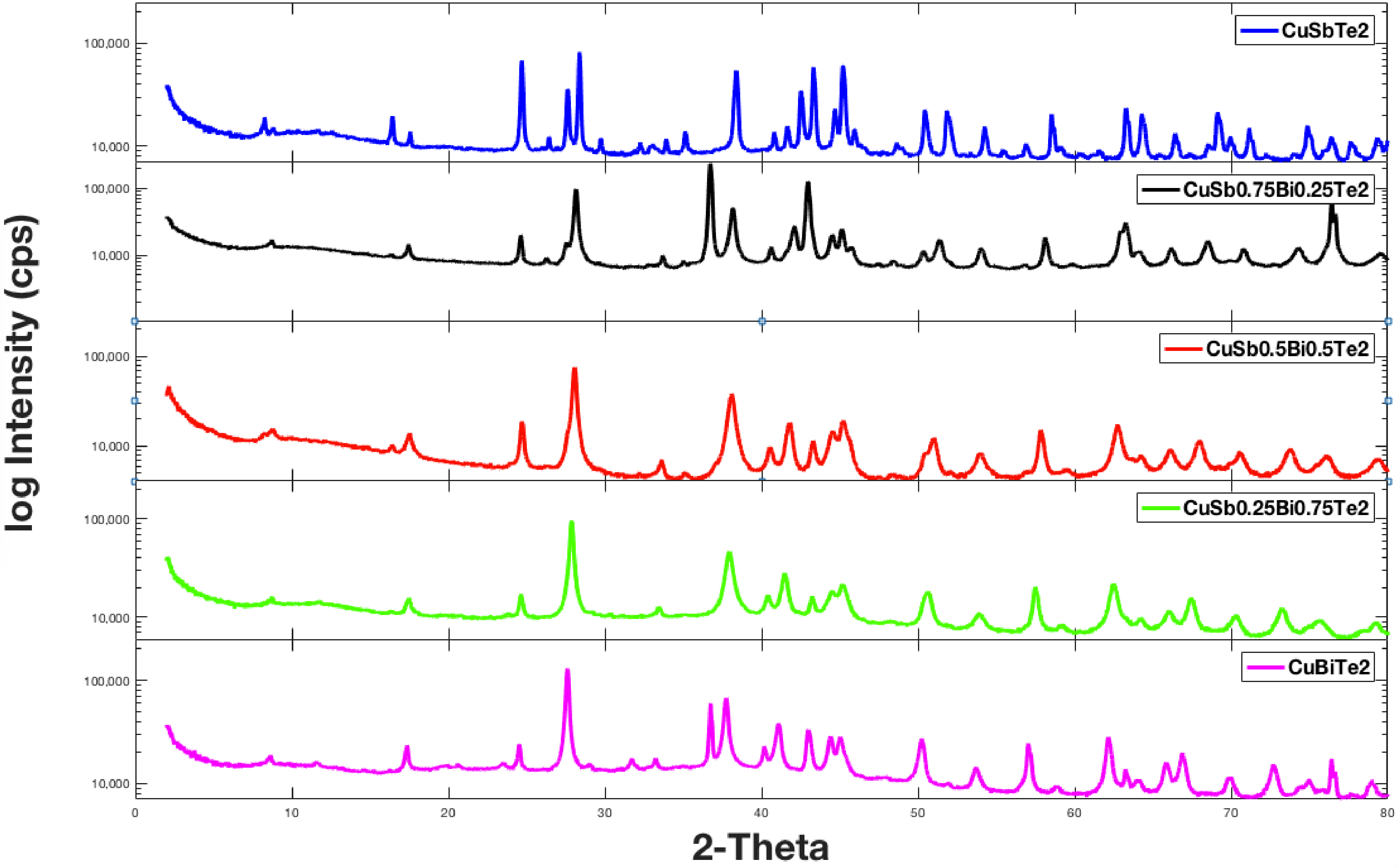
TE Figure-of-Merit: $$ZT = \frac{\sigma (S)^2}{(\kappa_e + \kappa_L)} . T$$

Thermal Conductivity

- A standard measure of the effectiveness of a thermoelectric material’s properties in the context of energy harvesting
- Not necessarily the best way to evaluate thermoelectric materials. It’s important to consider individual parts of zT as well, such as thermal conductivity and its overall influence on output power

Elements were weighted → Alloy was melt-quenched → Alloy was milled → Powder was spark plasma sintered

XRD

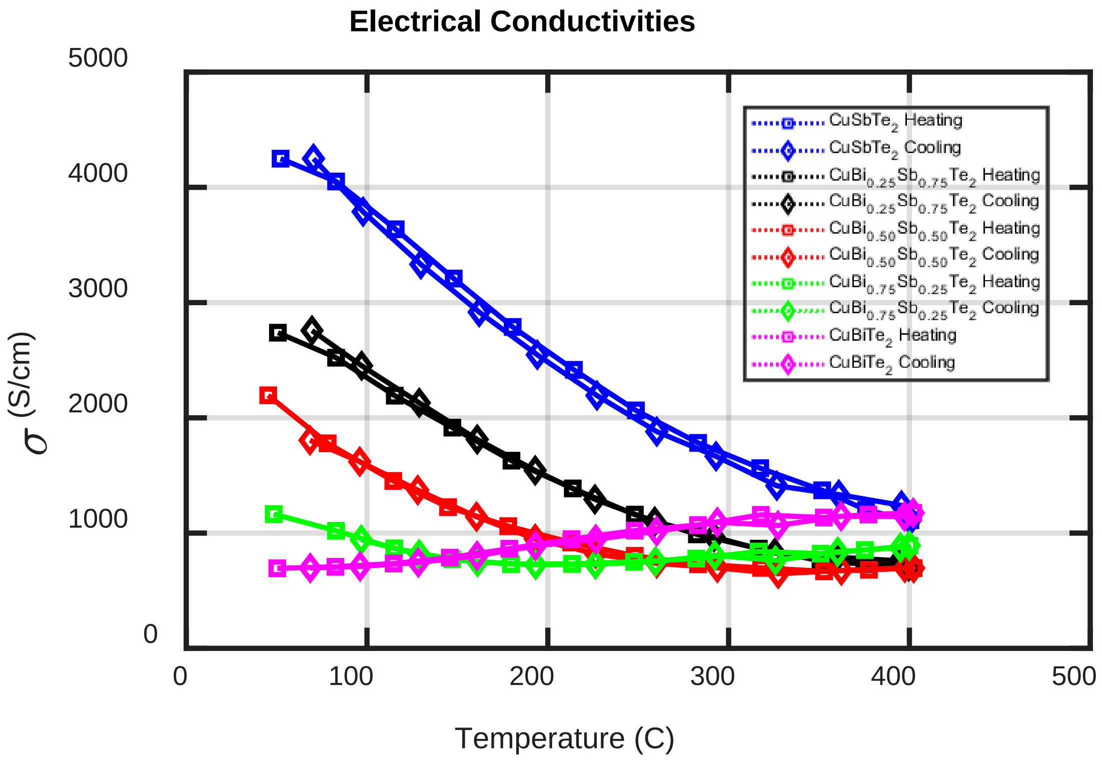


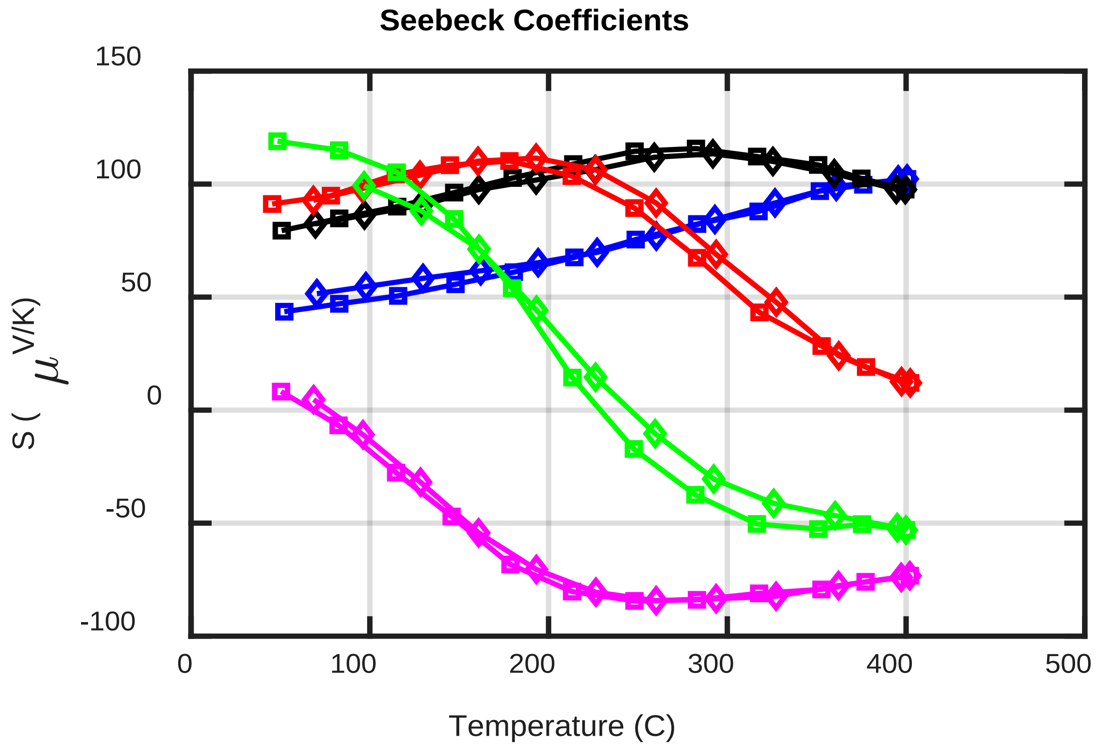
log Intensity (cps)
100,000
10,000
CuSbTe2
CuSb0.75Bi0.25Te2
CuSb0.5Bi0.5Te2
CuSb0.25Bi0.75Te2
CuBiTe2
0
10
20
30
40
50
60
70
80
2-Theta


A545 1280x1024 2018/07/05 10:58:04 Unit: mm Magnification: 15.3 x 1
DL0
L=8.277 mm
2.0 mm

LSR

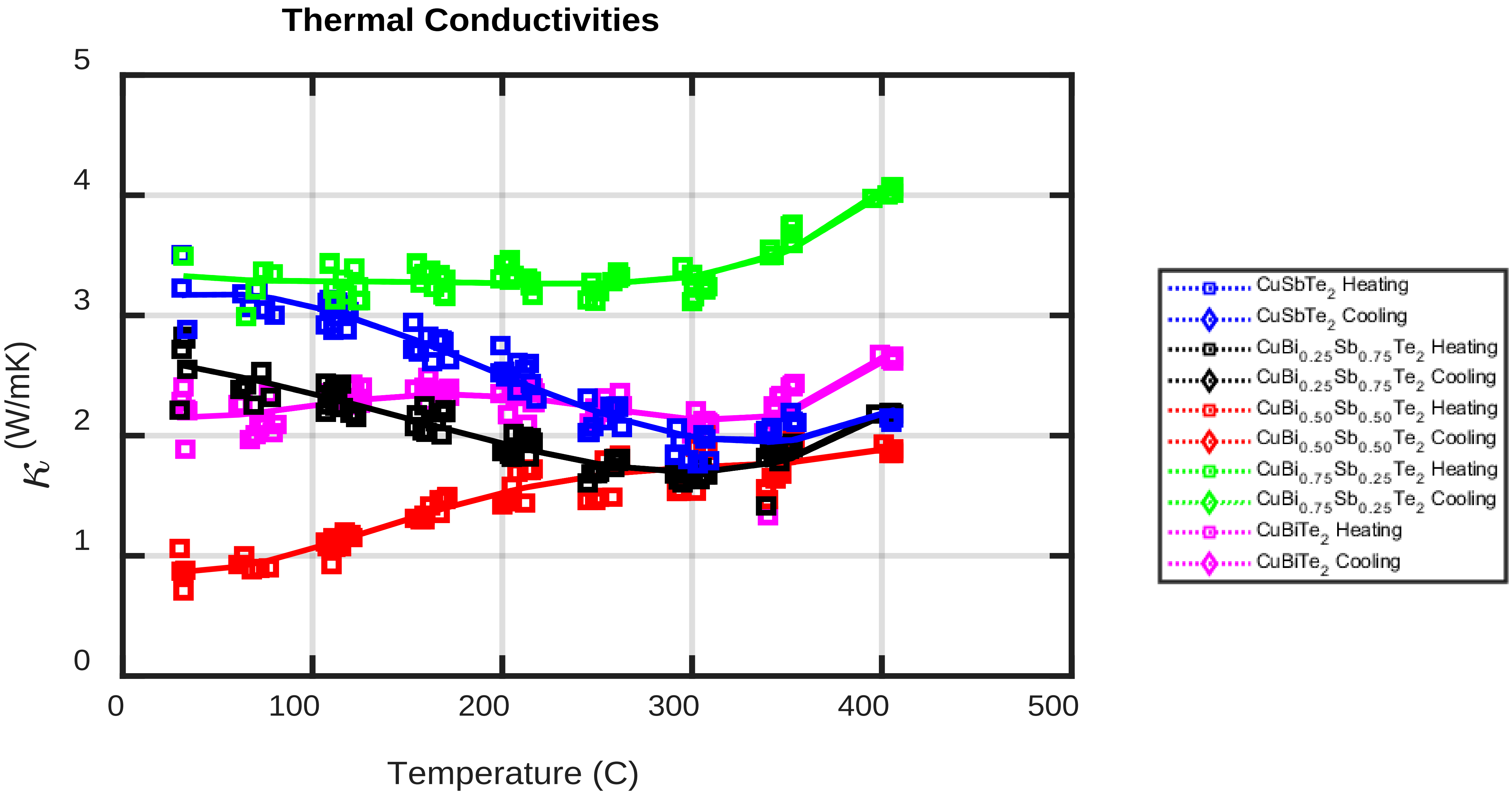
- A means to measure the Seebeck coefficient and electrical conductivity of a sample, typically a cylinder or bar of roughly 10 mm or greater
- Our temperature range: 40C to 400C
- Nuances:
  - Probes and how they make contact with the sample (two probes make contact with a single sample that is held by two gradient heaters)
  - Steps between gradient heating rates sometimes can be problematic depending on the thermal conductivity of a sample
  - Measurement must be taken with helium in the LSR due to good heat transfer


Electrical Conductivities
5000
4000
3000
2000
1000
0
σ (S/cm)
0
100
200
300
400
500
Temperature (C)
$CuSbTe_2$ Heating
$CuSbTe_2$ Cooling
$CuBi_{0.25}Sb_{0.75}Te_2$ Heating
$CuBi_{0.25}Sb_{0.75}Te_2$ Cooling
$CuBi_{0.50}Sb_{0.50}Te_2$ Heating
$CuBi_{0.50}Sb_{0.50}Te_2$ Cooling
$CuBi_{0.75}Sb_{0.25}Te_2$ Heating
$CuBi_{0.75}Sb_{0.25}Te_2$ Cooling
$CuBiTe_2$ Heating
$CuBiTe_2$ Cooling


Seebeck Coefficients
150
100
50
0
-50
-100
S (μV/K)
0
100
200
300
400
500
Temperature (C)

LFA

- A means to measure thermal diffusivity and eventually various components of thermal conductivity (predominantly electronic thermal conductivity and lattice thermal conductivity)
- Six samples can be measured at a time via laser flash measurements – very convenient and fast!
- Entire process takes place under vacuum, meaning that heating is somewhat difficult at times. Reasonable when going from 40C to 400C.



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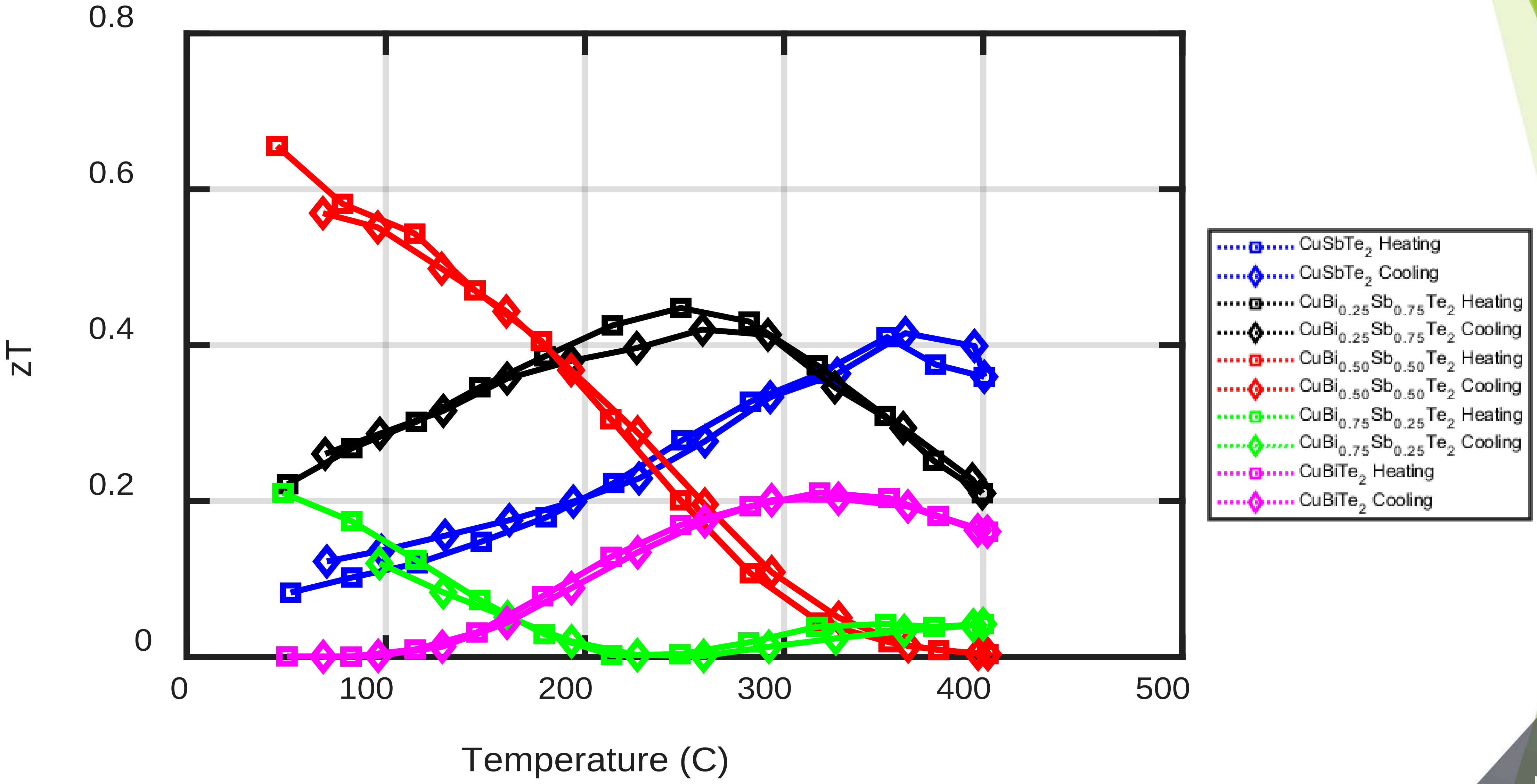
zT Figure of Merits



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Other Measurements

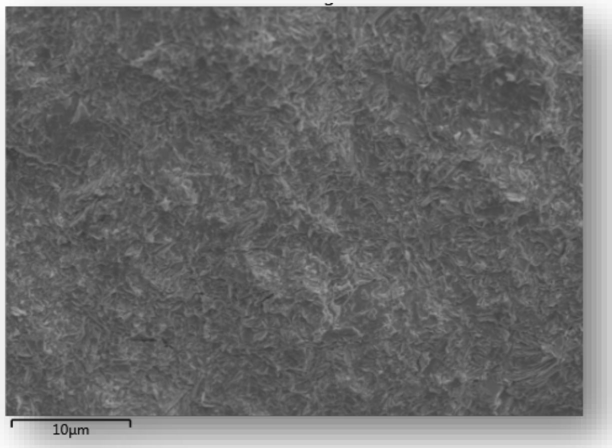
- Density measurements via a scale extension that utilizes Archimedes principle – provides precise density measurements
- DSC, or Differential Scanning Calorimetry, will be utilized for specific heat data in order to better calculate thermal conductivity

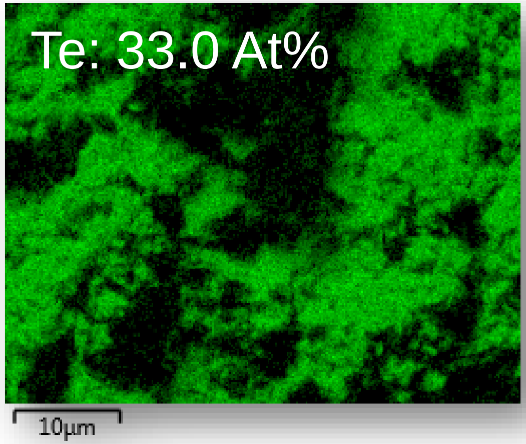
Thermal Conductivity

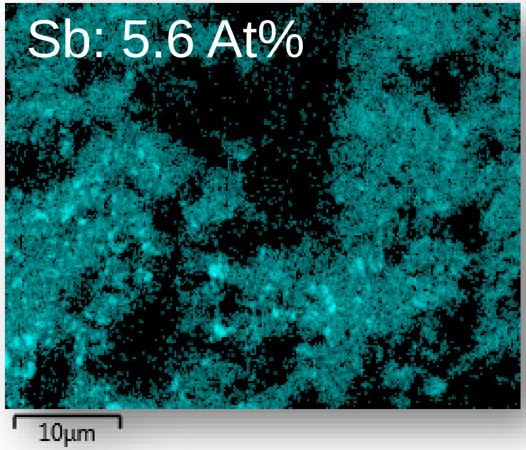
Thermal Diffusivity $$\alpha = \frac{\lambda}{\rho \; C_p}$$

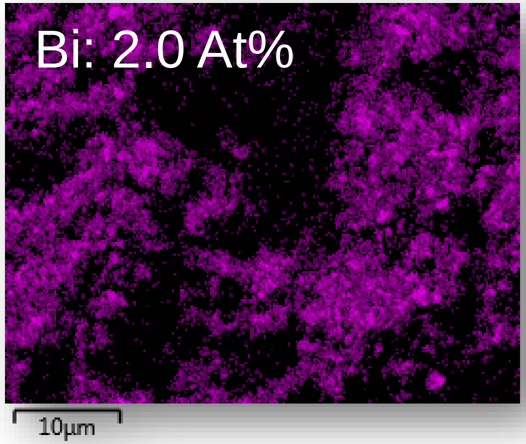
Density   Specific Heat Capacity

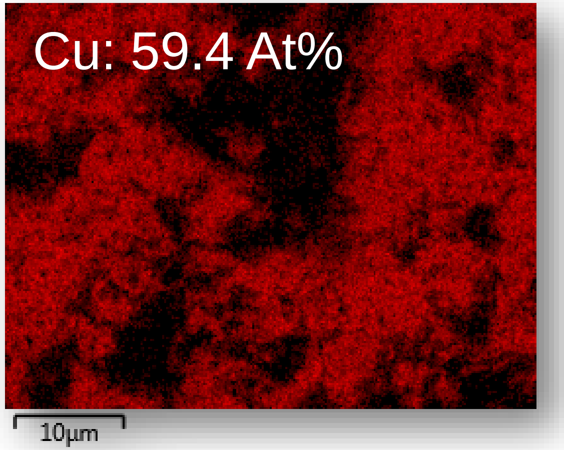
Energy Dispersive X-ray Spectroscopy in Scanning Electron Microscope











EDS scans confirmed the homogeneity of the synthesized $CuBi_{0.50}Sb_{0.50}Te_2$

Conclusions

- Of the compositions investigated, **$CuBi_{0.5}Sb_{0.5}Te_2$** proved to be the most interesting due to its **ultra-low thermal conductivity (~0.9 $Wm^{-1}K^{-1}$)** and resulting **zT of approximately 0.65 at 45^oC**
- Reason(s) for ultra-low thermal conductivity are yet unknown and **require(s) exploration**
- Samples will be made and analyzed for compositions around $CuBi_{0.5}Sb_{0.5}Te_2$, such as $CuBi_{0.4}Sb_{0.6}Te_2$ and $CuBi_{0.6}Sb_{0.4}Te_2$ for alloy optimization
- Further processing techniques will be introduced, such as **annealing and microwaving**, to further optimize the zT