Synthesis, Characterization, and Thermoelectric Properties of Copper Bismuth Sulphides

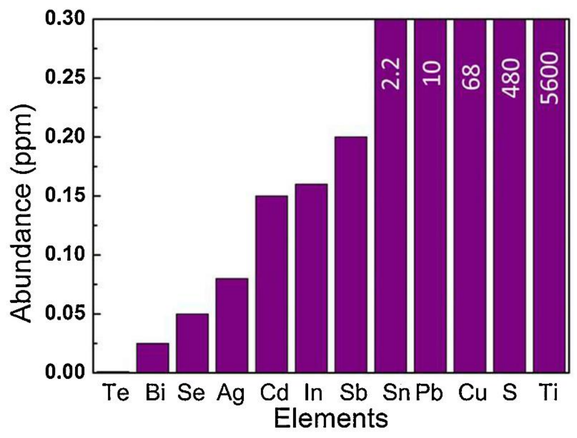
University of Reading

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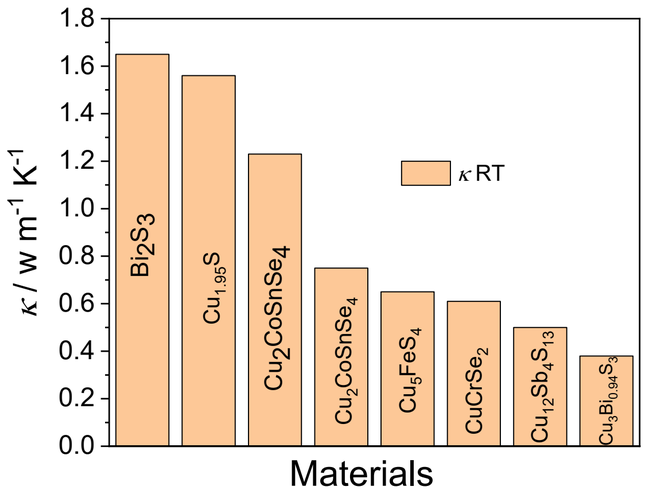
Dedicated to Prof Anthony Powell

Introduction

- Copper and sulphur are abundant and widely available in mineral ores.[1,2]

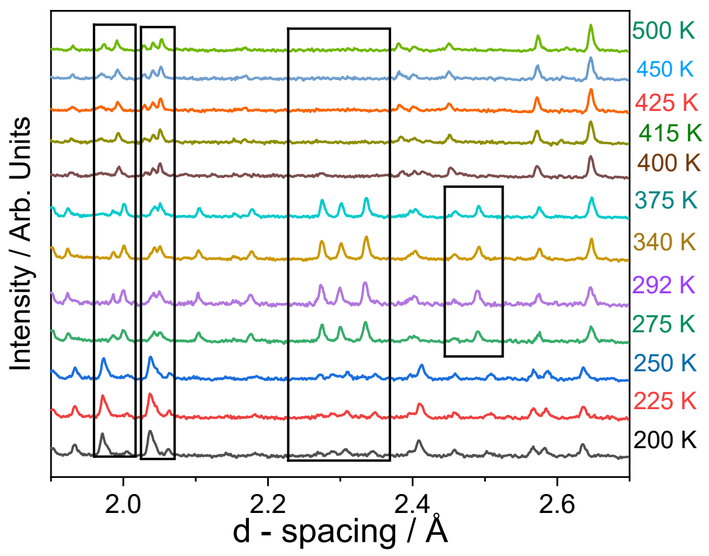


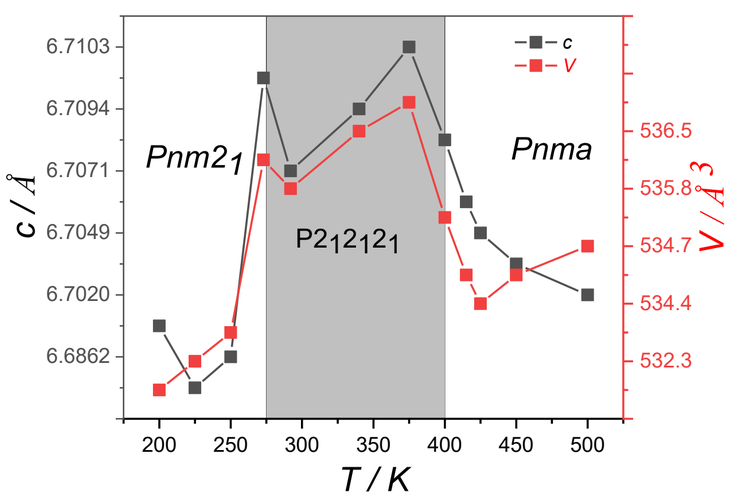
- Among Cu–S-based materials, $Cu_3Bi_{0.94}S_3$ exhibits the lowest thermal conductivity.

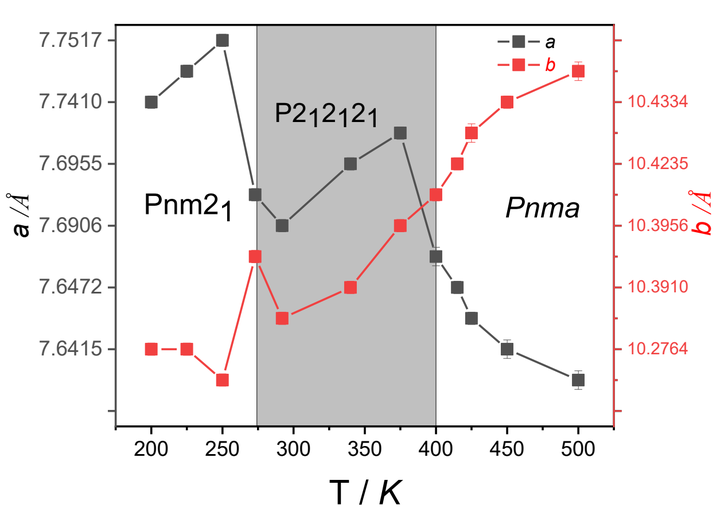


Neutron diffraction

- Phase transition from $Pnm2_1$ below RT to $P2_12_12_1$ at RT up to 380 K then *Pnma* above 400 K.
- Cu becoming disordered from 4-fold site at RT to 8-fold sites above 400 K.

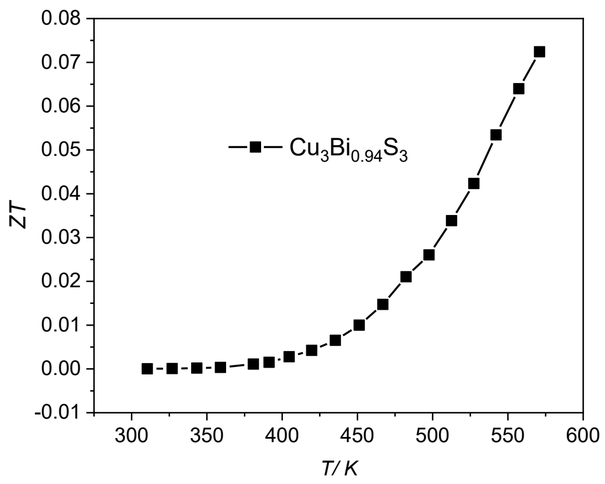


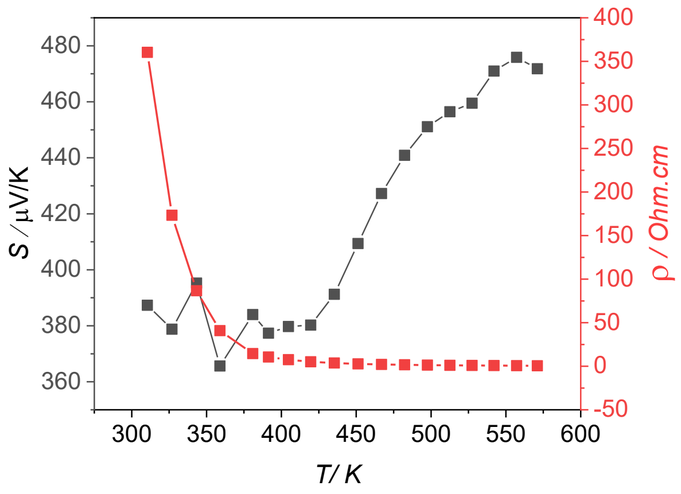




Thermoelectric properties

- At RT ρ is 350 Ωcm, and S is 390 $\mu V/K$.
- S increases with temperature ,and the positive value confirms p-type conduction.
- The maximum value of ZT is 0.07 at 550 K.



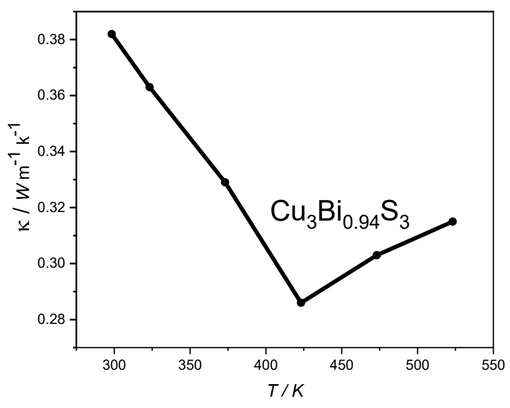


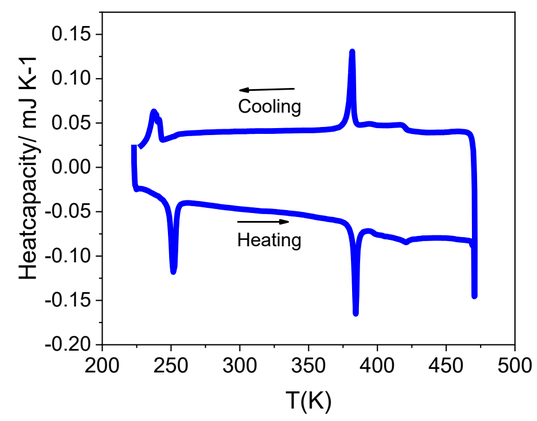
Conclusion

- The increase in κ is associated to a phase transition in which Cu becomes disordered.
- Crystal structure of low-temperature phase determined.

Objective

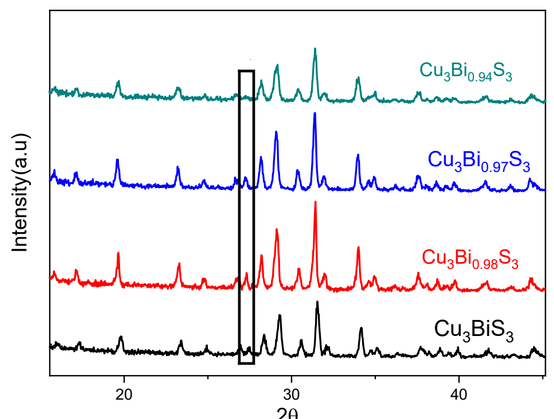
- K shows abnormal behaviour above 400 K.
- DSC show two phase transitions at 250 K and below 400 K



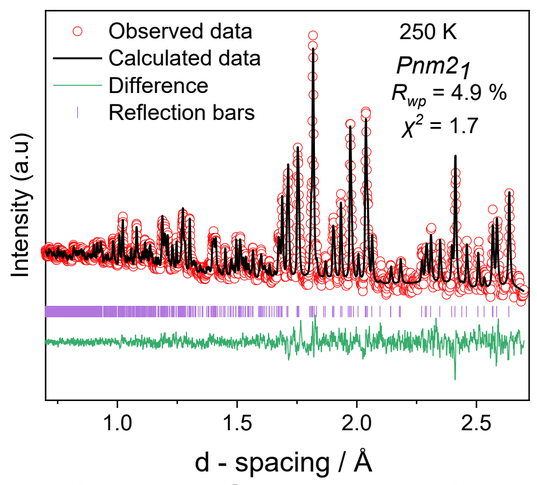


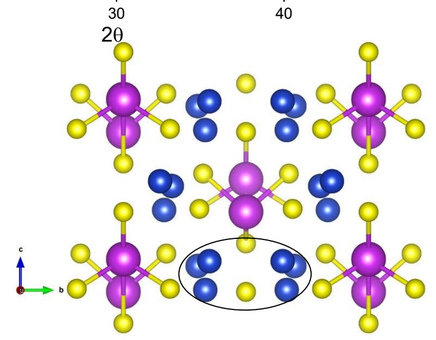
Synthesis

- High temperature method was used.
- Bi-impurity found.
- Pure phase made at $Cu_3Bi_{0.94}S_3$.

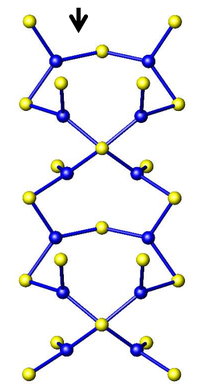


Rietveld refinement

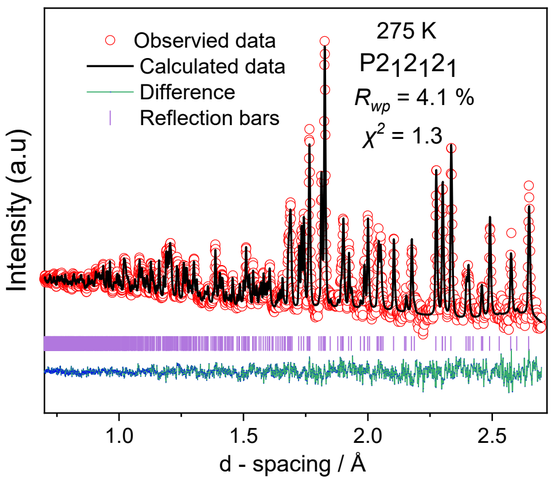


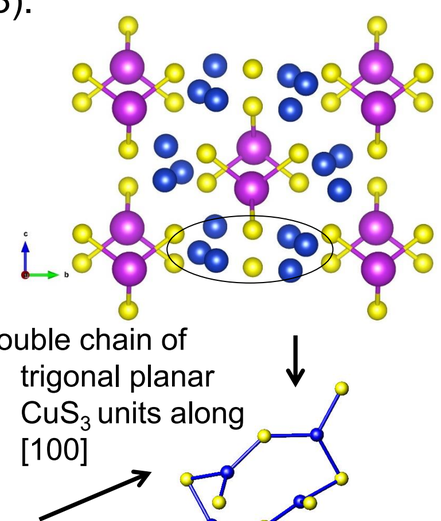


Double chain of trigonal planar CuS_3 units along [100]

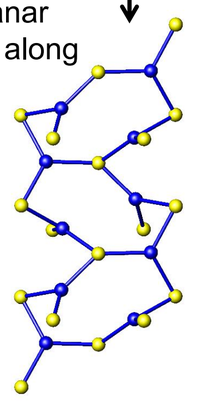


There are S atoms coordinated to 4 copper cations, and also with lower coordination numbers (2 and 3).

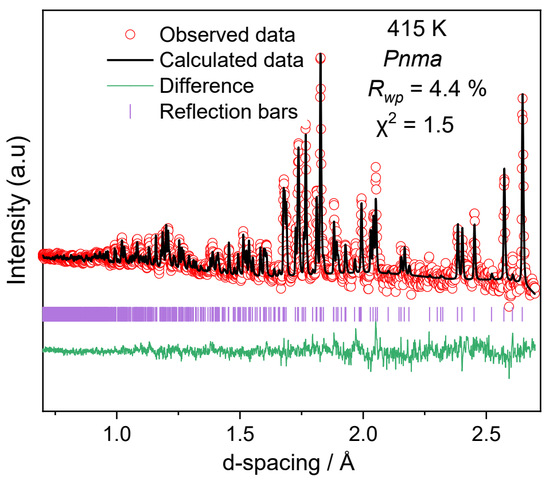


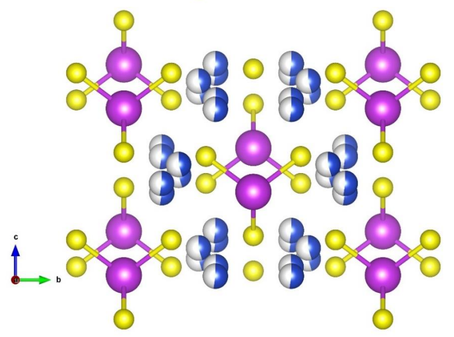


Double chain of trigonal planar CuS_3 units along [100]



All S atoms coordinated to 3 copper cations





References

1. A. V. Powell, *Journal of Applied Physics*, 2019, 126.100901.
2. Z.-H. Ge, L.-D. Zhao, D. Wu, X. Liu, B.-P. Zhang, J.-F. Li, J. He, *Mater. Today*, 2016, 19, 227–239.

Acknowledgments

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