Towards the efficient and sustainable preparation of thermoelectric materials

Marina Tabuyo Martínez[1], Marta María González Barrios[1], Manuel Cerro Carracedo[1], David Jiménez Merino[1], Óscar Juan Durá[2], Jesús Prado Gonjal[1]

[1] Inorganic Chemistry Department, Complutense University of Madrid, E-28040, Madrid, Spain
[2] Applied Physics Department, University of Castilla la Mancha, E-13071, Ciudad Real, Spain

* marinata@ucm.es ; jpradogo@ucm.es

MADRID 2022 – LVIII Congreso de la Sociedad Española de Cerámica y Vidrio

Overview

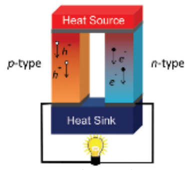
- Nowadays, the key is to find efficient and sustainable energy generation systems.
- Energy production and industrial processes produce waste heat as a sub-product.
- Waste heat can be converted into useful electrical energy by using thermoelectric devices.
- Commercial thermoelectrics show conversion efficiencies lower than 6 %.[1]
- An intensive search for novel materials, such as skutterudites and chalcogenides, is required.

Thermoelectricity

Conversion of a temperature gradient into electrical energy or viceversa.

$$zT = \frac{S^2}{\rho \cdot \kappa} T$$

zT: figure of merit
S: Seebeck coefficient (μV K^{-1})
ρ: electrical resistivity (Ω m)
κ: thermal conductivity (W m^{-1} K^{-1})
T: temperature (K)

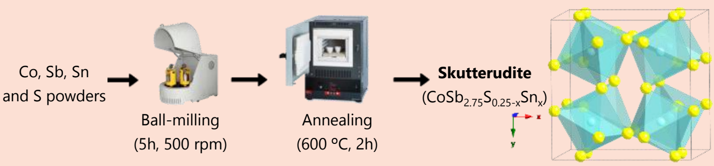


Freer et al. *J. Mater. Chem. C* **2020**, *8 (2)*, 441-463

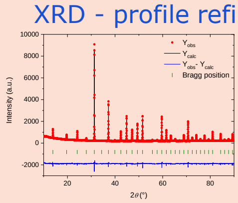
Alternative synthetic routes

- They offer many advantages, such as:
  - Higher control of the reaction.
  - More homogeneous and pure products.
  - Improved control of particle size and morphology.
  - Reduction of energy consumption.
- In this work, we have explored the following techniques:
  - Ball-milling.
  - Microwave-hydrothermal method.
  - Co-precipitation.

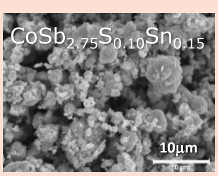
$CoSb_{2.75}S_{0.25-x}Sn_x$ (0.05 < x < 0.20) by ball-milling and short annealing



XRD - profile refinement $CoSb_3$

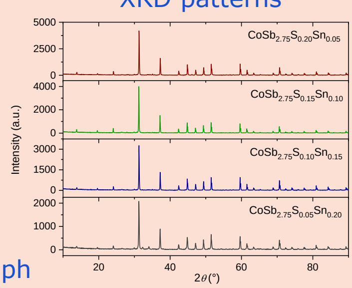


Cubic space group: *Im-3*
a = 9.0321(7) Å

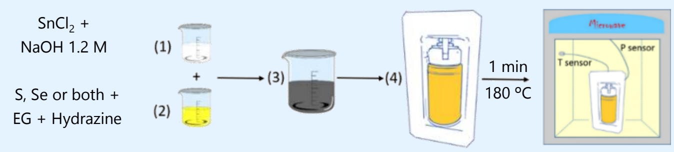


SEM micrograph

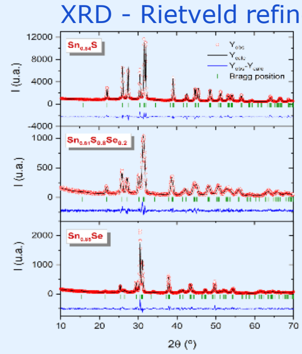
XRD patterns



SnQ (Q = S, Se) by microwave-hydrothermal method [2]



XRD - Rietveld refinements

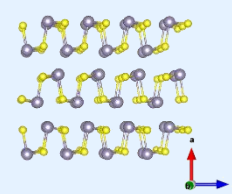


a = 11.2052(9) Å
b = 3.9867(3) Å
c = 4.3265(4) Å

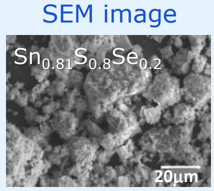
a = 11.3096(5) Å
b = 4.029(1) Å
c = 4.352(1) Å

a = 11.5151(7) Å
b = 4.1579(9) Å
c = 4.4328(9) Å

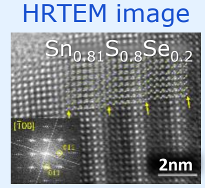
orthorhombic: *Pnma*



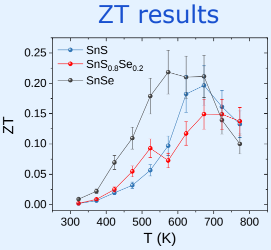
SEM image



HRTEM image

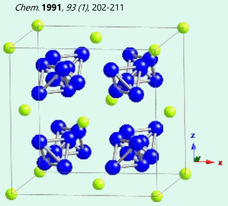


ZT results

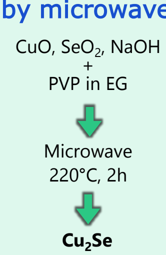


Cu_2Se by microwave-hydrothermal method

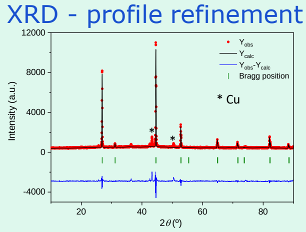
Yamamoto et al. *J. Solid State Chem.* **1991**, *93 (1)*, 202-211



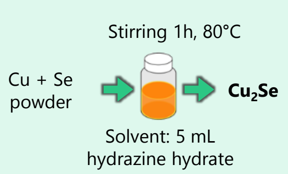
Cubic space group: *Fm-3m*
a = 5.7212(9) Å



XRD - profile refinement

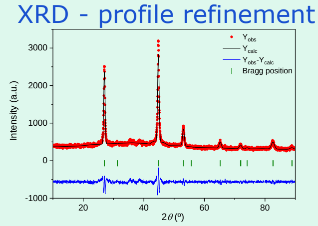


Cu_2Se by co-precipitation



Mulla et al. *ACS Sustainable Chem. Eng.* **2020**, *8 (37)*, 14234-14242

XRD - profile refinement



Conclusions

- A wide range of both traditional and novel thermoelectric materials can be prepared by alternative synthetic routes (ball-milling, microwave-hydrothermal, coprecipitation).
- These alternative preparation methods consume less energy, leading to more efficient and sustainable processes which are more likely to be compatible with large-scale production.
- Tunable thermoelectric properties are achieved by modifications in the synthetic pathways leading to tailored materials.

References

[1] Z. Ma et al. *Mater. Sci. Semicond. Process.*, **2021**, *121*.
[2] M. M. González-Barrios et al. *Ceram. Int.* **2022**, *48(9)*, pp. 12331-12341.

Acknowledgements. This work has been supported by the Madrid Government (**Community of Madrid- Spain**) under the Multiannual Agreement with **Complutense University** in the line Program to Stimulate Research for Young Doctors in the context of the V PRICIT (Regional Programme of Research and Technological Innovation): Project **PR65/19-22459**. This work has also been supported by the **Ministry of Science and Innovation** (Spanish Government): Project **PID2020-112848RB-C21**. Besides JPG and MMGB thanks to the **Community of Madrid** the granting of the **PEJ-202-AI/IND-17706** Research Assistant contract, through the Youth Employment Operational Program and the Youth Employment Initiative.