Establishing synthesis-composition-properties relationships for enhanced and reproducible thermoelectric properties of MgAgSb

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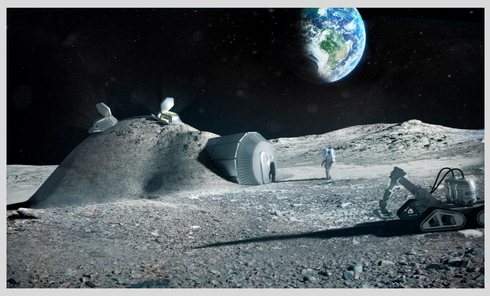
Motivation

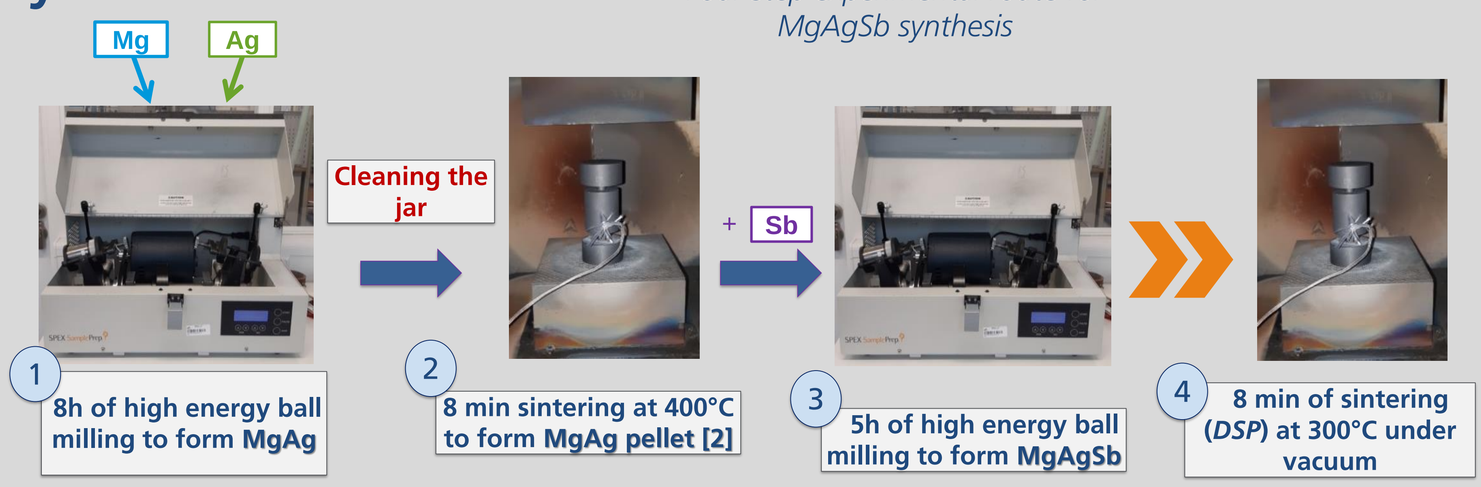
- Establish a long term and sustainable Moon base in the upcoming years (Artemis program)
- TEG would be a good way to provide, electricity on the Moon base due to the absence of moving parts and their reliability.
- α-MgAgSb working temperature range and mechanical properties make it a good candidate to withstand the conditions expected on the Moon.

Future lunar habitat [1]



Synthesis method

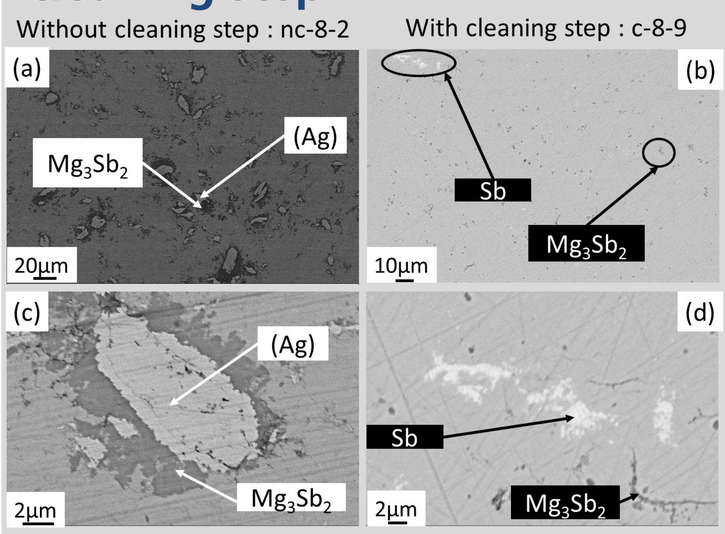
Four-step experimental route for MgAgSb synthesis



Aim

- Find the experimental route that gives the highest reproducible efficiency while being up-scalable at an industrial scale.
- Quantitative assessment of the impact of secondary phases on the TE properties

Results: effect of the cleaning step



- nc-8-2 (no cleaning step): Mg_3Sb_2 + *(Ag)*
- c-8-9 (cleaning step): Mg_3Sb_2 + *Sb*

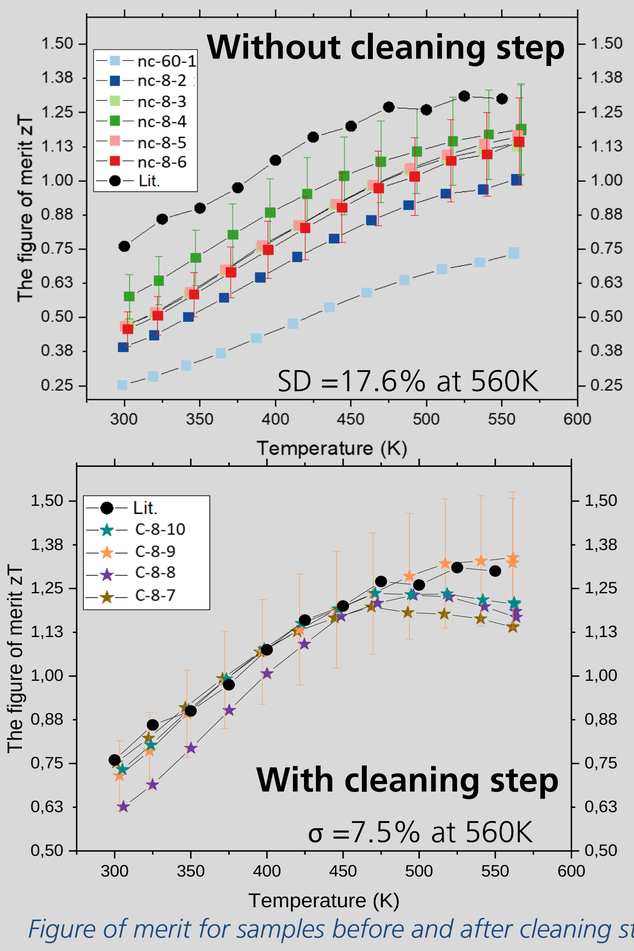


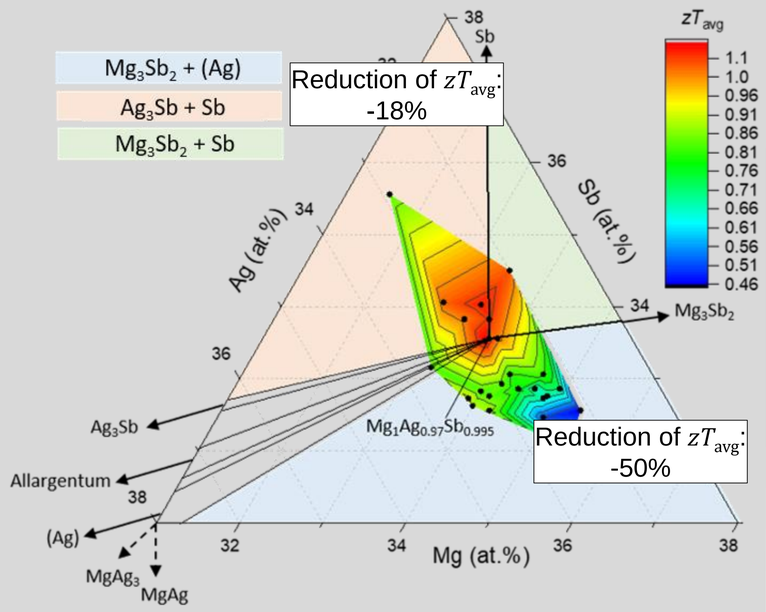
Figure of merit for samples before and after cleaning step

- After cleaning step → higher reproducibility of TE properties
- *zT* within the same range as literature

→ *Process control improved*

Discussion

Analysis of effective composition vs. TE properties



The average figure of merit versus the effective composition determined by EDX. Averaging range : T_c = 300 K; T_h = 550 K

- For a given deviation from the „ideal" stoichiometry:

zT_{avg} samples Sb-rich stoichiometry > zT_{avg} samples Sb-poor stoichiometry.

- Deviation between 1 and 2 at% in Mg and Sb from $MgAg_{0.97}Sb_{0.995}$ corresponds respectively to -50% and -20% in zT_{avg}

Single phase region estimation

- *Simple defect chemistry model* to provide a *rough* estimate for the phase width**:** no external dopant was employed → assume *p* is affected only by the MgAgSb matrix properties (V_{Ag} and Ag_{Mg})

- *p* defined as the hole density minus electron density. With Sb content remaining constant :

$$\Delta p = \frac{16\Delta x}{V}$$

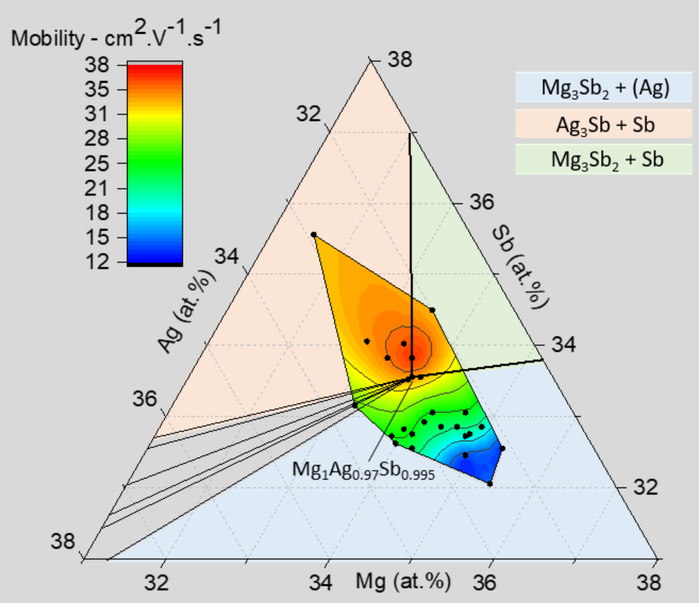
- For an observed maximum variation of $5 \cdot 10^{19}$ cm^{-3} between the samples:

$$MgAg_{0.97-\delta}Sb_{0.995} \; with \; \delta = 0.001$$

→ *Homogeneity range ~ 0.1 at% as upper limit*

- Almost all samples are outside the homogeneity range

→ *The observed changes in p are mainly due to secondary phases*



Charge carrier mobility versus the effective composition determined by EDX

- MgAgSb p-type semiconductor + Mg_3Sb_2 n-type impurity + (Ag) rich solution
  → decrease drastically *μ*, thus *σ* and *zT*
- *p-type MgAgSb + p-type Mg_3Sb_2 impurity + Sb* seems less detrimental for *μ*

Conclusion

Modified synthesis route:

- ✓ Improved the reproducibility of the TE properties between several batches
- ✓ Enhanced the achieved zT_{max} to 1.34 ± 0.19 at 561 K

? *Exact position of the single phase region not known*

? *Why do the different secondary phases affect so differently the TE properties*

References: [1] www.esa.int; [2] Rodriguez-Barber, I., et al., On the influence of AgMg precursor formation on MgAgSb microstructure and thermoelectric properties. Journal of Alloys and Compounds, 2021

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Scientific article can be found in Journal of Materials Chemistry A for more details

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