Poster

Fe-based skutterudite-like compounds

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Skutterudite is a mineral with the chemical formula $CoAs_3$ that crystallises in the space group $Im\ \bar{3}$ with a = 8.195(3) Å [1]. The structural analogue $CoSb_3$ (a = 9.036 Å) has always been of greater interest because of its higher electrical conductivity due to its less ionic Co-Sb bonds. However, this implies high thermal conductivity, which makes $CoSb_3$ unsuitable as a thermoelectric material. By filling the icosahedral voids in the structure of skutterudite-like compounds, the thermal conductivity can be significantly reduced but the high electrical conductivity is retained to a large extent, making these materials viable candidates for use as intermediate-temperature thermoelectric materials [2]. At the same time, the lattice parameter increases depending on the filling fraction and the filling atom.

To make a thermoelectric material viable for scale-up, rare or critical elements should be avoided. Therefore, alternative compounds using Fe instead of Co are more attractive. There are numerous compounds with sum formulae $M_yFe_4Sb_{12}$ (M = lanthanides, (earth) alkali metals, etc., y from 0 to 1) in literature [3], although thorough crystallographic analysis of most of these phases is lacking. We provide further insight into some Fe-based skutterudite-like phases based single-crystal structure analyses, e.g. with respect to ordering phenomena.

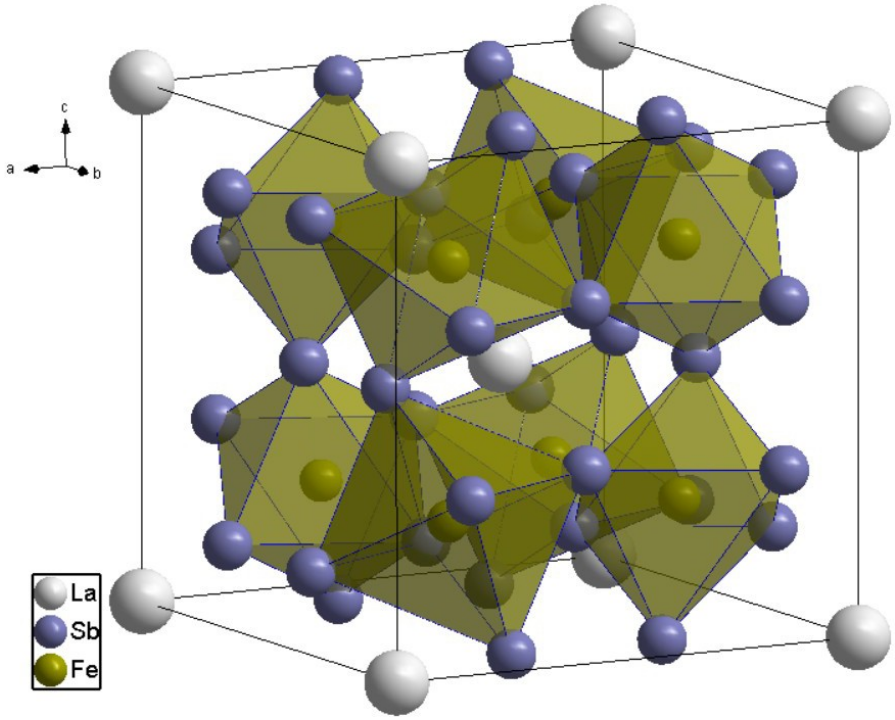

Figure 1. Structure of $La_{0.83}Fe_4Sb_{12}$.

[1] Mandel, N. & Donohue, J. (1971). *Acta Crystallgr. Sect. B* **27**, 2288-2289. doi:10.1107/S0567740871005727

[2] Liu, Z.-Y., Zhu, J.-L., Tong, X., Niu, S., & Zhao, W.-Y. (2020). *J. Adv. Ceram.*, **9**, 647–673. doi:10.1007/s40145-020-0407-4

[3] Tong, X., Liu, Z., Zhu, J., Yang, T., Wang, Y., & Xia, A. (2021). *Front. Mater. Sci..*, **15**, 317-333. doi:10.1007/s11706-021-0563-7

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