Thermophysical properties in the Kentrolite-Melanotektite family of compounds

New insights into the crystal-chemistry, mechanical properties and thermal expansion of Kentrolite and Melanotektite

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In Short

- DFT-simulations on the thermophysical properties to construct microscopic models for the thermal expansion
- Feasibility-screening of selective hypothetical compounds for synthesis
- Investigations into the negative linear compressibility in the Kentrolite-Melanotektite family of compounds

A satisfactory solution to the crystal structures of Melanotektite and Kentrolite was only found one century (1991)[1] after the original discovery of Kentrolite in 1880[2].

The structure type is tolerant to isostructural substitution, allowing for the incorporation of diverse elements into the host lattice [3,4]. In 2003 another closely related oxide, β-$PbAlBO_4$ (**Fig. 1**), was published[5], further expanding the chemistry.

While much progress has been made on the chemistry of these long-known materials, information on the physical properties is still scarce. In 2018 we initiated a project to explore these compounds for their scientific potentials. The focus of our investigations is on the thermophysical properties, with particular emphasis on the thermal expansion. The mechanisms underlying our experimental observations are elucidated using Density functional theory (DFT).

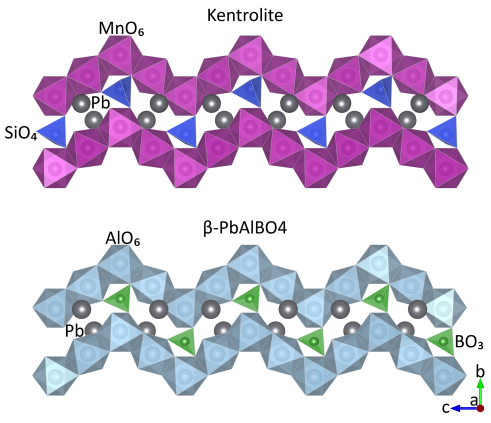

***Figure 1:** Zig-zag-chain structure motives in $Pb_2M_2T_2O_9$-type materials (top) and β-$PbAlBO_4$ (bottom).*

In our unpublished work on β-$PbAlBO_4$ (**Fig. 1**) we experimentally found axial negative thermal expansion (ANTE) and the far more rare phenomenon of negative linear compressibility (NLC)[6]. These properties are potentially useful in temperature-adaptive optical coatings and effectively incompressible structures, respectively. Using the resources of a HLRN-"*Schnupperkennung*", we were able to reproduce this behaviour computationally and shed light on the microscopic origin of the phenomena.

Our preliminary results suggest a typical wine-rack structure motive[7] (**Fig. 2**) to be responsible for the NLC-phenomenon. This purely mechanical feature is also closely linked to the ANTE observed in the same compound. Based on this success we are committed to further investigate this fascinating structure type.

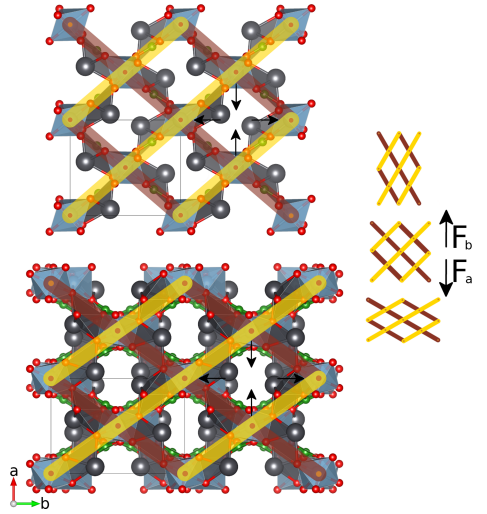

***Figure 2:** Chain-link fence structure motive in α-$PbAlBO_4$ (top) and β-$PbAlBO_4$ (bottom) schematically superimposed on renderings of the crystal structures.*

In addition to explaining the elastic and thermophysical properties we intend to replace the toxic lead with non-toxic Bi(III) and Sn(II) in these compounds. Since the field of possible candidates is too large to explore without any pre-selection, DFT-simulations would guide us in choosing appropriate compositions for our synthetic work.

WWW

https://www.ckfs.uni-bremen.de/Arbeitsgruppe/Murshed.htm

More Information

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Project Partners

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