



Institute of Thermomechanics, Czech Academy of Sciences

invites you to a lecture within the lecture series **Institute of Thermomechanics Seminar**

Beyond Composition: How Structure and Processing Govern Functional Materials

prof. Patricia Almeida Carvalho

Department of Sustainable Energy Technologies at SINTEF (Oslo, Norway)

Understanding functional materials increasingly requires resolving how composition, crystal structure and processing-induced defects interact across multiple length scales. Here, advanced transmission electron microscopy, complemented by spectroscopy, diffraction, data-driven analysis and first-principles calculations, is used to address these relationships in semiconductor and thermoelectric materials.

In B-implanted cubic silicon carbide (3C-SiC), investigated as a potential intermediate-band solar absorber, STEM reveals a temperature-dependent evolution from point-defect clusters to stacking faults, dislocation networks and B-rich $B_{13}C_2$ precipitates. These precipitates trap B up to 1773 K, whereas at higher temperature increased solubility suppresses precipitation, enabling dopant concentrations of $\sim 10^{19} \text{ cm}^{-3}$ at 1873 K.

In the emerging class of high-entropy semiconductors, the crystal structure of (Zn,Mn)(Fe,Co,Ni)Sb is resolved by combining atomically resolved STEM-EDS with energy-filtered CBED. This approach distinguishes between closely related half- and full-Heusler structures that cannot be reliably discriminated by conventional X-ray diffraction because of the similar scattering factors of the constituent transition metals.

Finally, microscopy provides the physical basis for interpreting a data-driven analysis of thermoelectric tetrahedrites comprising more than 8,000 literature datapoints. Combined with targeted experiments and DFT, the analysis shows that variations in reported properties are governed less by dopant identity than by processing-induced microstructure, particularly consolidation quality and porosity associated with gas evolution during sintering.

Together, these studies illustrate how advanced electron microscopy can connect local chemistry and structure with macroscopic functionality, revealing dopant precipitation, crystallographic ordering and processing-induced microstructure as decisive factors in the design of functional materials.

**The lecture will be held on Friday, October 2nd, 2026 at 10:00 a.m.
in the building of the Institute of Thermomechanics (Lecture Hall),
Dolejškova 5, 182 00 Prague 8**

Contact persons: Hanuš Seiner, Dušan Gabriel