Structure – property studies; intermetallics and functional oxides

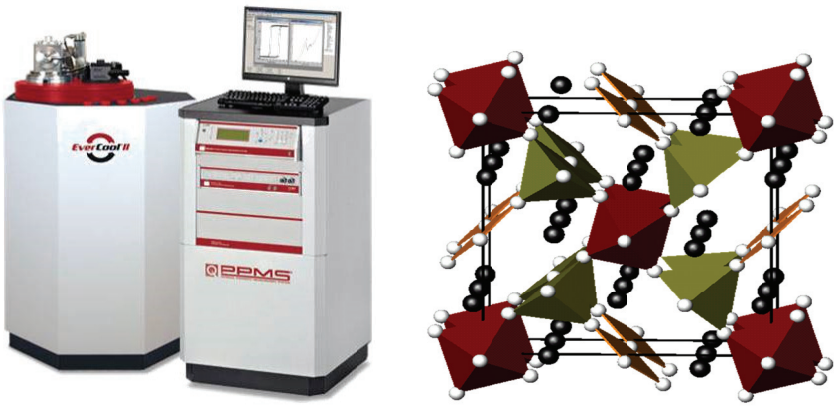
In this project you will combine methods like X-ray or neutron diffraction that enables determination of the atomic arrangement of crystalline solids, with chemical/physical characterization methods. The objective is to identify and understand the interplay between chemistry, crystal structure and emerging properties (that eventually are those critical for a given application). Such insight can open for tuning of properties or synthesis of novel materials with high performance. This is highly relevant for future materials for energy storage and conversion, chemical processing, sensors and many other applications. The project will involve extensive use of advanced instrumentation in the RECX X-ray lab at KI, experiments at the European Synchrotron in Grenoble, neutron diffraction at IFE, Kjeller, and participation in ongoing projects with partners in Scandinavia and Europe. The experimental studies may be combined with DFT modeling if desired.

Examples of this:

- Can new properties emerge in perovskite oxides with platina group cations?
- What atomic arrangements can provide high Li-/Na-ionic transport for use in batteries?
- How can electronic properties of oxides be modified via introduction of other anions?
- How can magnetostructural transitions provide efficient solids for refrigeration?
- How can the activity of Co-oxide based catalysts be enhanced by substitutions?
- How can II-VI semiconductors be modified by dopants or via solid solutions?
- How and why do properties change from bulk to nanoparticles to ultrathin coatings?

What you will learn:

- To use advanced tools in X-ray (and neutron) scattering for structure determination
- Synthesis methods for either oxides or intermetallics
- To characterize physical properties, study thermal stability, or catalytic activity
- To design and build special equipment; and use modern software for data analysis
- Become a key part of the Nafuma team and work closely with the researchers



Example of instrumentation: physical property measurement system (PPMS) for measuring of magnetization. Resistivity, heat capacity, thermal conductivity (left); crystal structure of an oxide with three types of different coordination polyhedra with transition metal cations, yielding special magnetic and electronic interactions (right).

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