Abstract for the general public

Project's title: Entropy engineering and interface optimization in materials for highly effective thermoelectric energy conversion

Motivation

Global climate change, environmental pollution, and increase in energy costs are urgent issues faced by modern society. Thermoelectric (TE) energy conversion, in concert with other emerging energy technologies, can contribute to a sustainable energy supply. TE devices are simple by design, scalable from μW to kW; due to the absence of mechanically moving parts they are silent in operation and have a long lifetime free of maintenance. Waste heat recovery by TE generators (TEG) may thus reduce the consumption of fossil fuels and the emission of CO_2. However, exploitation of TEG yet remained limited due to moderate efficiency, cost barriers for a mass application not yet passed and a delay in material-specific joining technologies for devices, but also concern on sustainability because of involvement of toxic elements. The development of lightweight TE materials, as pursued here, will facilitate the use of TE technologies in mobile applications (automotive, aerospace). Argyrodites and magnesium silicide-based solid solutions are promising TE materials to respond to these challenges.

Project goal

The project aims to develop highly effective thermoelectric materials from the families of argyrodites and magnesium silicide-based solid solutions, qualifying them for usage in cheap and eco-friendly energy converters. To achieve the goal of the project, we propose the following strategies:

1. Exploitation of the **Entropy Engineering (EE)** approach for enhancement of the energy conversion efficiency through effective optimization of electronic structure.
2. Utilization of **internal interface effects** in nanocomposite materials for enhancement of the TE properties through the polycrystallinity and multiphase nature.
3. **Identification of the origin of electrical and thermal resistances** in TE material to metal electrode interfaces for further improvement of the efficiency of thermoelectric converters.

Description of the research

Within the project, we will investigate two promising families of thermoelectric materials, i.e. argyrodites and silicides. The main aspects of the research can be listed as follows: i) preparation and characterization of argyrodite and silicide-based materials, ii) investigation of the internal interfaces, iii) analyses of the external interfaces, and iv) assembling of thermoelectric unicouple for verification of the energy conversion efficiency. During the project, we will apply local transport measurement on a nano-scale to do the best possible optimization of properties.

The expected results

The main outcome of the project will be the highly efficient lightweight and low-cost argyrodite and silicide-based materials suitable for the construction of the TE converters. Within the project, we plan to offer and verify a few novel concepts for the enhancement of thermoelectric properties. Particularly, the combined effect of entropy engineering, internal and external interfaces will be tested for the investigated materials.