25th International Conference on
ADVANCED NANOSCIENCE AND NANOTECHNOLOGY
May 06-07, 2022 | Webinar

Received date: 17-04-2022 | Accepted date: 21-04-2022 | Published date: 24-05-2022

Structural evolution and correlation with thermoelectric properties in various materials

Norbert M. Nemes
Universidad Complutense de Madrid, Spain

A good thermoelectric material must have a high Seebeck coefficient (S), be a good electrical conductor, and be a good thermal insulator. The efficiency of a thermoelectric is commonly characterized by its thermoelectric figure of merit, zT=σS2T/κ. Thermoelectrics could play an important role in saving energy in the future, sustainable, economy, if only they had a zT>4. Today, the best materials, commercial highly doped semiconductors, do not exceed by much zT ~ 1, while state-of-the-art zT reported very recently in materials such as SnSe, GeTe or skutterudites do not exceed zT ~ 2.5. The electrical (σ) and thermal (κ) conductivity in metals is tied by the Wiedemann-Franz law. However, κ also has an important contribution in semiconductors due to the vibrations of the crystal lattice. There are several strategies pursued to improve thermoelectric properties, including the so-called "phonon glass, electric crystal" (PGEC) with great prominence. It is based on decreasing κlatt in different ways while preserving the good electronic properties (S and σ).

We use several, far from equilibrium, synthesis methods to obtain thermoelectric materials with promising properties. We characterize the static and dynamic structure with neutron scattering and synchrotron X-ray diffraction, with Rietveld refinement analysis to obtain both the crystalline structure and the dynamics of the constituent atoms through thermal factors (atomic displacement parameters).

We correlate this structure with the thermoelectric properties, in particular with the contribution of the crystalline network to the thermal conductivity in families of materials of SnSe and its alloys with various metallic elements, alloys of Bi2Te3 with Sb and Se, and skutterudites of CoSb3 filled with rare earth and alkali or alkaline earth atoms. In this talk several results of these material families will be described, always aiming to establish correlations between the structural peculiarities with the observed properties.

Recent Publications

1. Norbert M Nemes, Javier Gainza, Federico Serrano-Sánchez, João EFS Rodrigues, Yves Huttel, Oscar J Dura, Michael M Koza, María Teresa Fernández-Díaz, Juan J Meléndez, Bence G Márkus, Ferenc Simon, José Luis Martínez, José Antonio Alonso, (2020)"High-Performance n-type SnSe Thermoelectric Polycrystal Prepared by Arc-Melting",Cell Reports Physical Science (12) 100263
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4. .Norbert M Nemes, Mirko Rocci, Dhavala Suri, Akashdeep Kamra, Gilvânia Vilela, Yota Takamura,Jose L Martinez, Mar Garcia Hernandez, Jagadeesh S Moodera (2020) "Large enhancement of critical current in superconducting devices by gate voltage" Nanoletters 21 (1) 216-221
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Biography

Norbert M. Nemes is an experimental solid-state physicist who obtained his Ph.D. in Physics from the University of Pennsylvania in 2002 after postdoctoral stays in the NIST Center for Neutron Research and also the Materials Science Institute of Madrid he is a Professor of Applied Physics at the Universidad Complutense de Madrid, one of the largest and oldest Spanish universities. He has published over 100 research papers with an h-index of 22 on topics ranging from materials of reduced dimensions, superconductors, spintronics, and magnetic anisotropy, multifunctional materials (magnetoelectric coupling), and in the last years on thermoelectrics.

nmnemes@ucm.es