KN-24

Complexity of crystal structures and properties of thermoelectric materials

Yuri Grin[1]
[1]*Max-Planck-Institut Für Chemische Physik Fester Stoffe, Dresden, Germany*
E-mail: grin@cpfs.mpg.de

Complexity of the crystal structures is one of the key issues in the further understanding of the structure-dependent physical behaviors – in particular thermoelectric properties - of materials. It is well accepted approach for realization of good thermoelectric materials which suggests the use of elements with atomic masses, large carrier mobility and compounds with large unit cells (complex crystal structures) for reducing the thermal conductivity and controlling the electronic transport [1]. Being a philosophical category for the description of the state of the mind, complexity is not easy to be straight forward quantified. Structural complexity of compounds may be described in several ways, e.g. on base of the crystallographic features of materials (number of atoms in the unit cell or symmetry), or considering chemical and crystallographic order/disorder, or taking into account thermodynamic factors (phase diagrams, formation reactions), etc. According to crystallographic description, a special family of materials – the so-called complex metallic alloys or phases (CMA) – was defined in order to shed more light on the influence of their unusual crystal structures on the chemical and physical properties [2]. Experimental studies on single crystals revealed that neither electronic nor thermal transport behaviors follow strictly the crystallographic understanding of structural complexity. As a promising results in this direction, recently was shown that the reduced lattice thermal conductivity of type-I clathrates without vacancies and with respect to such with ordered vacancies suggests that disordered vacancies disturb the heat transport more efficient as the electronic transport. Further insights into the phonon transport are achieved considering the complexity of appearance and spatial separation of regions with different chemical bonding in the context of the structural complexity. Inhomogeneity and anisotropy of chemical bonding support the reduction of the thermal conductivity in dependence of crystallographic direction [3].

[1] Slack, G. A. (1995) In: Thermoelectric Handbook. Ed. D. M. Rowe .CRC, Boca Raton, FL 407ff.
[2] Steurer, W. Dshemuchadse, J. (2016) Intermetallics. Oxford University Press.
[3] Ormeci A. et al. (2015) J. Thermoelectr. № 6, 16-32.

Keywords: crystal structure, chemical bonding, thermoelectric properties