Oral Contributions

[MS28] Energy-related Materials
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[MS28-01] Structural features of thermoelectric materials. Grin, Y.

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Intermetallic compounds are a large family of inorganic materials which are recently actively studied in respect of their thermoelectric properties. Several crystallographic features reflect their structural complexity which is considered as one of the factors of the influence on thermoelectric behavior.

Structural complexity of thermoelectric materials may be discussed taking into account either their crystallographic characteristics like point symmetry, number of atoms per unit cell, or considering chemical and positional order/ disorder, or – finally - including phase diagrams, formation conditions [1]. A special family of intermetallic compounds – the so-called complex metallic alloys (CMA) – was defined employing the crystallographic description [2,3].

In particular for the cage compounds with the characteristic structural features, structural complexity opens an opportunity to influence more directly the thermal conductivity separating - at least partially – its lattice and electronic parts. It was shown that the reduced lattice thermal conductivity of $Ba_8Ni_{3.5}Ge_{42.1\square 0.4}$ with respect to defect-less Ba–Ni–Ge type-I clathrates and with respect to $Ba_8Ge_{43\square 3}$ with ordered vacancies suggests that disordered vacancies hinder efficiently the heat transport [4].

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[3] J. Dshemuchadse, W. Steurer. MRS Proc. **1517** (2012) kk01.
[4] L. T. K. Nguyen et al. Dalton Trans. **39** (2010) 1071.