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CRYSTALLOGRAPHY AND THERMAL CONDUCTIVITY OF THERMOELECTRIC CLATHRATES

Yuri Grin
Max-Planck-Institut fur Chemische Physik fester Stoffe, Germany

Since their first discovery in 1965 [1] the intermetallic clathrates attracted attention of materials scientists, chemists and physicists in particular due to their fascinating crystal structures, especially the formation of large cavities within the three-dimensional framework which are usually occupied by filler species [2]. These cavities may be also un-occupied (empty clathrates [3]). From the point of view of chemical bonding, three types of atomic interactions are present in this family of inorganic materials: polar and non-polar covalent interactions in the framework, ionic forces and strongly polar covalent dative bonds between the filler atoms in the cavities and the framework [4]. The coexistence of the different bond kinds (inhomogeneity of the bonding) causes the reduced thermal conductivity and opens the possibility to tune the charge carrier concentration, which makes these materials interesting for thermoelectric applications. The combination of the electronic and phononic transport in clathrates suitable for thermoelectric application was recognized and proven quite early [5,6]. One of the challenges on the way to an application is the preparation of large amounts of the material with reproducible properties, and its control by the up-scaling of the manufacture processes, due to the complexity of the phase diagrams [7]. Another challenge is the understanding of the low thermal conductivity of this family of materials One possible mechanism is associated with the presence of low-energy non-dispersive optical phonons caused by vibrations ('rattling') of the filler atoms within the cage-like crystal structure [8,9]. Recently was shown, that these optic modes of the fillers hybridize with that of the framework, and there are no indications for the formation of isolated oscillators in the system. Moreover, the low thermal conductivity is characteristic also for the empty clathrates. A new phonon-filter mechanism was proven by the inelastic neutron scattering experiments [10,11].

grin@cpfs.mpg.de