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Crystal Structures and Thermoelectric Properties of A8Al8Si38 (A = K, Rb and Cs)

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Intermetallic clathrates with the host-guest type structures attract an interest as perspective materials for thermoelectric applications. Recently, they were also proposed as possible materials for solar energy conversion [1] and as anode materials for lithium ion batteries [2-3]. The intermetallic clathrates are mainly formed by the group IV elements as the host atoms and alkaline or alkaline earth metals as the guests with the latter being the majority [4]. Particularly, the host framework can be formed by the partial substitution of group 14 elements by group 13 elements or transition metals.

We have prepared A8Al8Si38 clathrates (A=K, Rb and Cs) [5] by a combined flux method that allows to obtain pure samples as crystalline gray powders. The crystal structures of these compounds were studied using high-resolution neutron powder diffraction. The neutron scattering experiments were performed on the powder diffractometer SPODI at the research reactor FRM-II (Garching, Germany). The Rietveld refinements of the crystal structures were carried out using the FullProf package [6]. The distribution of Al atoms in the framework as obtained from neutron data was additionally confirmed by solid state 27Al-MAS NMR. Thermoelectric properties were investigated on the cold pressed pellets prepared in a High Pressure Multi-Anvil apparatus. The resistivity, thermal conductivity and Seebeck coefficient were measured in the temperature range from 2 to 400 K.

Studied compounds A8Al8Si38 possess type-I clathrate structure and crystallize in the cubic space group $Pm^{-}3n$ and lattice parameter a = 10.48914(6) Å, 10.53163(7) Å and 10.58734(7) Å for K8Al8Si38, Rb8Al8Si38 and Cs7.9Al7.9Si38.1, respectively. All host positions in the framework show mixed occupancy by Al and Si, but their distribution slightly varies depending on the type of guest atoms. All A8Al8Si38 clathrates are n-type semiconductors with a relatively low thermal conductivity and a high Seebeck coefficient.

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