Synthesis of clathrate $K_8Ga_{x-y}Al_ySi_{46-x-y}$ with enhanced thermoelectric property

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Inorganic clathrates are excellent candidate for high-performance functional materials in various applications such as thermoelectrics and photovoltaics [1-3]. We report here synthesis and thermoelectric properties of polycrystalline clathrates $K_8Ga_{x-y}Al_ySi_{46-x-y}$. X-ray diffraction patterns indicated that the products are the target phases and contain only a trace level of secondary phase. Spark plasma sintering was carried out to obtain dense specimens for compositional and physical property characterizations. Chemical compositions of the spark plasma sintered products determined using electron probe micro-analysis were found to be $K_{7.6(1)}Ga_{7.9(4)}Si_{39.9(6)}$ (KGaSi), $K_{7.6(1)}Ga_{4.9(1)}Al_{3.0(8)}Si_{39.4(8)}$ (KGaAlSi), and $K_{7.6(1)}Al_{7.0(4)}Si_{39.3(2)}$ (KAlSi). Electrical conductivity measurement below 320 K indicated semiconducting behavior for KGaSi and KGaAlSi samples and metallic behavior for KAlSi sample. Seebeck coefficient measurement confirmed *n*-type conduction for all the samples. Compared with the end phases KGaSi and KAlSi, almost two-fold enhanced value of figure of merit (*ZT*) was obtained for the intermediate compound KGaAlSi. With respect to KGaSi, improved electrical conductivity and reduced thermal conductivity along with slightly decreased Seebeck coefficient are responsible for the enhancement of the *ZT* in KGaAlSi.

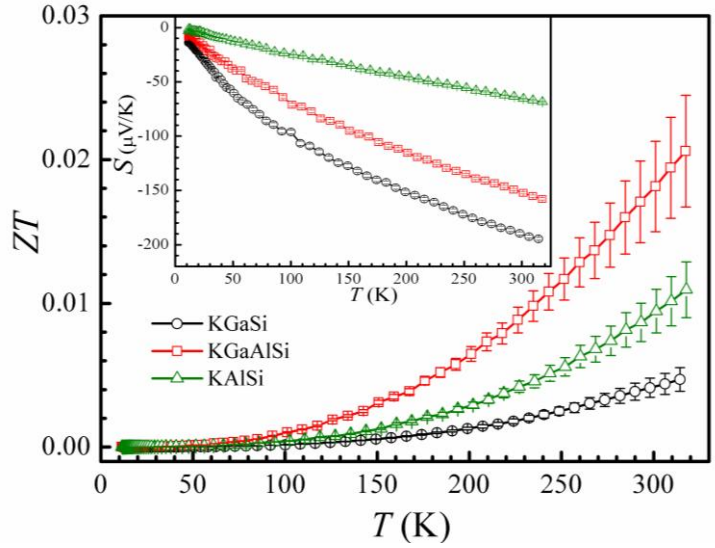

Figure 1: *ZT* with temperature. Inset shows variation of Seebeck coefficient.

References:

[1] M. Christensen, S. Johnsen, B. B. Iversen, Dalton Trans. 39, 978-992, (2010).

[2]Y. He, G. Galli, Nano Lett.14 2920-2925 (2014).

[3] M. Imai, A. Sato, H. Udono, Y. Imai, H. Tajima, Dalton Trans. 40, 4045-4047 (2011).