

## Structure characterization of $\text{Sr}_8\text{Ga}_{16}\text{Ge}_{30}$ and $\text{Ba}_8\text{Ga}_{16}\text{Ge}_{30}$ clathrate with single crystal neutron diffraction

D. Yu<sup>1</sup>, M. Tayebjee<sup>1</sup>, R. Piltz<sup>1</sup>, K. Cai<sup>2</sup>, L. Wong<sup>1</sup>, A. Stampfl<sup>1</sup>

<sup>1</sup>*Bragg Institute, ANSTO, Menai, NSW, Australia*

<sup>2</sup>*Functional Materials Research Laboratory, Tongji University, Shanghai 200092 PR China., Shanghai, China*

The key consideration in the development of more efficient thermoelectric materials is to design materials that conduct heat like a glass but maintain good crystal-like electrical conductivities, that is to design so called phonon glass and electron crystals (PGEC's), as proposed by Slack [1]. One potential PGEC are clathrates that consist of a cage framework of the group 13/14 elements and alkali, alkaline earth or rare earth atoms trapped within the cages. The properties of such clathrates strongly depend on the details of their structures, the dynamic disorder of the trapped atoms as well as the distribution of framework atoms.

The structure of single crystals of  $\text{Sr}_8\text{Ga}_{16}\text{Ge}_{30}$  and  $\text{Ba}_8\text{Ga}_{16}\text{Ge}_{30}$  are characterized by single crystal neutron diffraction, as a function of temperature. The general gallium-doped germanium cage structure with strontium or barium guest atoms inside is confirmed. The lattice constants are 10.704(1) Å and 10.759(2)Å for  $\text{Sr}_8\text{Ga}_{16}\text{Ge}_{30}$  and  $\text{Ba}_8\text{Ga}_{16}\text{Ge}_{30}$  respectively. Refinement shows that the gallium framework atoms preferentially occupy the 6c site and avoid the 16i site. For the guest atoms of Sr and Ba in the 24-atom cage, the split-site model (24k or 24j) is applied for the  $\text{Sr}_8\text{Ga}_{16}\text{Ge}_{30}$  structure while the single-site model (6d) is more applicable for the  $\text{Ba}_8\text{Ga}_{16}\text{Ge}_{30}$  structure. Thermal properties of Debye temperature, Einstein temperature and thermal conductivity have been extracted from the temperature dependence of atomic displacement parameters (ADPs).

(1) G. A. Slack, in CRC Handbook of Thermoelectrics, Edited by D. M. Rowe (CRC Boca Raton, FL, 1995), pp 407-440