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PII: S0022-4596(17)30246-3  
DOI: <http://dx.doi.org/10.1016/j.jssc.2017.06.025>  
Reference: YJSSC19843

To appear in: *Journal of Solid State Chemistry*

Received date: 8 May 2017  
Revised date: 17 June 2017  
Accepted date: 23 June 2017

Cite this article as: Jiefei Fu, Xianli Su, Yonggao Yan, Wei Liu, Zhengkai Zhang, Xiaoyu She, Ctirad Uher and Xinfeng Tang, Thermoelectric properties of Cu/Ag doped type-III Ba<sub>24</sub>Ge<sub>100</sub> clathrates, *Journal of Solid State Chemistry*, <http://dx.doi.org/10.1016/j.jssc.2017.06.025>

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# Thermoelectric properties of Cu/Ag doped type-III Ba<sub>24</sub>Ge<sub>100</sub> clathrates

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**Abstract:** Type-III Ba<sub>24</sub>Ge<sub>100</sub> clathrates possess low thermal conductivity and high electrical conductivity at room temperature and, as such, have a great potential as thermoelectric materials for power generation. However, the Seebeck coefficient is very low due to the intrinsically high carrier concentration. In this paper, a series of Ba<sub>24</sub>Cu<sub>x</sub>Ge<sub>100-x</sub> and Ba<sub>24</sub>Ag<sub>y</sub>Ge<sub>100-y</sub> specimens were prepared by vacuum melting combined with the subsequent spark plasma sintering (SPS) process. Doping Cu or Ag on the Ge site not only suppresses the concentration of electrons but it also decreases the thermal conductivity. In addition, the carrier mobility and the Seebeck coefficient increase due to the decrease in the carrier concentration. Thus, the power factor is greatly improved, leading to an improvement in the dimensionless figure of merit  $ZT$ . Cu-doped Ba<sub>24</sub>Cu<sub>6</sub>Ge<sub>94</sub> reaches the maximum  $ZT$  value of about 0.17 at 873 K, while Ag-doped Ba<sub>24</sub>Ag<sub>6</sub>Ge<sub>94</sub> attains the dimensionless figure of merit  $ZT$  of 0.31 at 873 K, more than 2 times higher value compared to un-doped Ba<sub>24</sub>Ge<sub>100</sub>.

Graphical Abstract

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