Accepted Manuscript

Enhanced thermoelectric performance in Cu_2GeSe_3 via (Ag,Ga)-co-doping on cation sites

Ruifeng Wang, Ang Li, Tianyu Huang, Bin Zhang, Kunling Peng, Hengquan Yang, Xu Lu, Xiaoyuan Zhou, Xiaodong Han, Guoyu Wang

PII: S0925-8388(18)32819-6

DOI: 10.1016/j.jallcom.2018.07.318

Reference: JALCOM 47034

To appear in: *Journal of Alloys and Compounds*

Received Date: 10 May 2018

Revised Date: 26 July 2018

Accepted Date: 28 July 2018

Please cite this article as: R. Wang, A. Li, T. Huang, B. Zhang, K. Peng, H. Yang, X. Lu, X. Zhou, X. Han, G. Wang, Enhanced thermoelectric performance in Cu_2GeSe_3 via (Ag,Ga)-co-doping on cation sites, *Journal of Alloys and Compounds* (2018), doi: 10.1016/j.jallcom.2018.07.318.

Enhanced Thermoelectric Performance in Cu_2GeSe_3 via (Ag,Ga)-co-doping on cation sites

Ruifeng Wang[a,d#], Ang Li[b#], Tianyu Huang[a,d], Bin Zhang[c], Kunling Peng[a,c], Hengquan Yang[c], Xu Lu*[c], Xiaoyuan Zhou[c], Xiaodong Han[b], Guoyu Wang*[a,d]

a. Chongqing Institute of Green and Intelligent Technology, Chinese Academy of Sciences, Chongqing 400714, P. R. China
b. Beijing Key Laboratory of Microstructure and Property of Advanced Materials, Beijing University of Technology, Beijing 100124, P. R. China
c. College of Physics, Chongqing University, Chongqing 401331, P. R. China
d. University of Chinese Academy of Sciences, Beijing 100044, P. R. China
#: these authors contribute equally to this work
Email address: guoyuw@cigit.ac.cn, luxu@cqu.edu.cn

Abstract

An enhancement on thermoelectric performance of Cu_2GeSe_3 *via* simultaneously Ag-alloying on Cu sites and Ga-doping on Ge sites is achieved. The relatively high solubility (~ 10%) of Ag on Cu sites allows for the strong point defect scattering for phonons, which causes remarkable reduction in lattice thermal conductivity. Ag-rich precipitates emerge when the amount of Ag is higher than the solubility on Cu site, which however do not have significant effect on the lattice thermal conductivity since it is already very close to the lower limit of kinetic theory. Ga-doping, an effective way to tune the hole concentration, leads to optimization of power factor in the whole temperature range. The maximal zT obtained in $Cu_{1.9}Ag_{0.1}Ge_{0.997}Ga_{0.003}Se_3$ is 1.03@786 K, about 58% higher than that in previous report. In addition, the average zT in the temperature range from 320 K to 786 K is 0.58, implying great potential for fabrication of thermoelectric devices.

Keywords: Thermoelectrics, Cu_2GeSe_3, Precipitates, Alloying, Doping