Enhancement of thermoelectric figure-of-merit in a wide temperature range in $\text{In}_4\text{Se}_{3-x}\text{Cl}_y$ bulk crystals

JONG-SOO RHYEE, Kyung Hee University, KYUNGHAN AHN, KYU HYOUNG LEE, Samsung Advanced Institute of Technology, JI HOON SHIM, Pohang University of Science and Technology, JAE HOON KIM, Yonsei University, KYUNG HEE UNIVERSITY TEAM, SAMSUNG ADVANCED INSTITUTE OF TECHNOLOGY COLLABORATION, POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY COLLABORATION, YONSEI UNIVERSITY COLLABORATION — Recently, we proposed that the charge density wave is a new pathway for high thermoelectric performance in bulk crystalline materials [1,2]. Through the quasi one-dimensional lattice distortion (Peierls distortion) in $\text{In}_4\text{Se}_{3-x}$ bulk single crystals, we have achieved a high thermoelectric figure-of-merit $ZT$ of 1.48 at 705 K. From the Boltzmann transport calculation, it was confirmed that the reported $ZT$ could be further increased if we could increase the chemical potential of the $\text{In}_4\text{Se}_{3-x}$ crystals. Here we report the significant increase of $ZT$ over a wide temperature range from 50 $^\circ$C to 425 $^\circ$C by chlorine doping in the $\text{In}_4\text{Se}_{3-x}$, which comes from the improvement of crystal quality and increase of chemical potential, resulting in the power factor enhancement and the thermal conductivity reduction.


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