**High-Performance Bi2Te3 Thermoelectric Materials *via* Modulation of Carrier Concentration Guided by SPB Model**

*Yuan WangA, Jin ZouB,C, Zhi-Gang ChenA,B*

A Centre for Future Materials, University of Southern Queensland, Springfield central, Australia;

B Materials Engineering, The University of Queensland, Brisbane, Australia;

C Centre for Microscopy and Microanalysis, The University of Queensland, Brisbane, Australia.

**Abstract**

Thermoelectric materials, enabling the direct conversion between thermal and electrical energies, have been considered as energy-saving alternatives for sustainable power generation. Due to the intrinsic interdependence of thermoelectric parameters, including electrical conductivity, Seebeck coefficient, and electrical thermal conductivity, modulation of carrier concentration (*n*) is of vital significance to obtain thermoelectric materials with high energy conversion efficiency, which is gauged by a dimensionless figure of merit *zT*. Here, we utilize the single parabolic band (SPB) model to predict the optimal *n* (~ 1 × 1019 cm-3) of bismuth telluride (Bi2Te3), and guide our experimental design. By reducing *n* from ~ 1 ×1020 cm-3 in the intrinsic Bi2Te3 to ~ 6 ×1019 cm-3 in the Cr introduced Bi2Te3, *zT* was effectively improved from 0.7 to 1.08 at 470 K, and high average *zT* close to 1 was achieved from 300 K to 470 K.

C:\Users\uqywan68\Desktop\Picture1.tif

**Figure 1.** Calculation results of SPB model showing the effective *zT* enhancement with reduced *n*.

**References**

1. Wang, Y.; Liu, W.-D.; Gao, H.; Wang, L.-J.; Li, M.; Shi, X.-L.; Hong, M.; Wang, H.; Zou, J.; Chen, Z.-G. (2019). High Porosity in Nanostructured *n*-Type Bi2Te3 Obtaining Ultralow Lattice Thermal Conductivity. ACS Appl. Mater. Interfaces, 11, 31237-31244.

2. Wang, Y.; Yang, L.; Shi, X.-L.; Shi, X.; Chen, L.; Dargusch, M.; Zou, J.; Chen, Z.-G. (2019) Flexible Thermoelectric Materials and Generators: Challenges and Innovations. Adv. Mater., 31, 1807916.