Carrier concentration optimization and Band convergence of $Mg_2Si_{1-x}Sn_x$ thermoelectric materials[1] XINFENG TANG, Wuhan University of Technology, WEI LIU, University of Michigan, XIANLI SU, Wuhan University of Technology, CTIRAD UHER, University of Michigan, XINFENG TANG TEAM, CTIRAD UHER TEAM — In our research, the optimization of electron concentration and the tuning of conduction band structure are explored in order to push it for application in power generation. Systematical experiments indicate that the appropriate over-stoichiometry of Mg content is beneficial to the adjustment of electron concentration in n-type $Mg_2Si_{1-x}Sn_x$ solid solutions. Moreover, the electron concentration of $Mg_2Si_{1-x}Sn_x$ is validly controlled by doping Sb or Bi with the combination of proper over-stoichiometry of Mg. First-principles calculations of the band structure and plentiful experimental researches proved that the bottom of the conduction band of $Mg_2Si_{1-x}Sn_x$ is characterized a double band structure, including a heavy band and a light band which converged in energy with the increase of the Sn/Si ratio and further degenerated at x = 0.65 ∼ 0.68. Consequently, the convergence and degeneration of two conduction bands give rise to remarkable elevation on the carrier effective mass and Seebeck coefficient without a detrimental effect on the carrier mobility, and therefore lead to a largely enhanced power factor. Due to the optimization of both the electron concentration and conduction band structure, n-type $Mg_2Si_{1-x}Sn_x$, being provided with electron concentration in the range of $1.6 \times 10^{20} \sim 2.5 \times 10^{20}$ cm^{-3} and x = 0.6 ∼ 0.7, show the highest ZT values of 1.3 at around 725 K and average ZT values about 1.0 within 500 ∼ 800 K.

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