A multiscale approach to enhance the thermoelectric properties of α-$SrSi_2$

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Abstract

Conventional thermoelectric materials such as Bi_2Te_3 have the best performances at room temperature and can reach a ZT about 1. However, the cost, the toxicity and the scarcity of Te limit the application of thermoelectric materials in the low temperature range (300 – 600K). The use of eco-friendly elements such as silicides alloys could overcome these concerns. Among them Mn-Si and Mg2(Si,Sn) reached a maximum figure of merit of 0.63 (723 K) and 0.8 (650 K) respectively [1,2] and α-$SrSi_2$ reaches a ZT about 0.15 at 300K which is the highest value for a silicide alloy at this temperature. The power factor of α-$SrSi_2$ is close to that of Bi_2Te_3 however its thermal conductivity (~5 W/m.K) limit its performances. In this work, we investigate the effect of the nanostructuring, Sr purity and substitution on the thermal and thermoelectric properties of α-$SrSi_2$ combining different metallurgical techniques [3,4]. We have shown that the nanostructuring by ball milling leads to an increase of the unit cell and of the concentration of defects which both modify the electronic band structure and phonon scattering. With this approach the lattice thermal conductivity contribution was decreased close to that expected to highly disordered or amorphous materials without impacting much the power factor. This multi scale approach enabled to improve the figure of merit to about 60% compared to our bulk reference.

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