Poster Presentation

Thermoelectric properties of new Co-Sb-Se system

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Energy is the linchpin for the growth of every developing country. To address the global energy supply, power conservation and energy management, generation of electricity from waste-heat resources attains more consideration. Developing and deploying affordable energy solutions and implementation of new energy technologies will develop society to achieve extraordinary affluence. Thermoelectric (TE) materials can directly convert the waste heat into electrical energy, which have the impending play in energy preservation and power generation [1]. The efficacy of the thermoelectric materials is often assessed by dimensionless figure of merit $ZT = \sigma S2/\kappa elec+ \kappa lat$, where σ is the electrical conductivity, S is the Seebeck coefficient (thermopower), $\kappa elec$ is the electronic part of thermal conductivity and $\kappa latt$ is the lattice part of the thermal conductivity.

Transition metal(TM) -based pnictides and chalcogenides are been widely studied due to their interesting properties in superconductor and thermoelectrics [2]. Invention of novel materials with complex structure will be of great interest in this field. Such materials of having complex and disorder structures comprise scatter phonons, ensuing in a low thermal conductivity particularly lattice part. Here we report the Co-Sb-Se, a new phase thermoelectric material having low band gap to find potential TE applications. The ternary compound of Co-Sb-Se system crystallizes in the orthorhombic space group Pnnm (60), with a unit cell containing 6 atoms. The structure contains 2 independent crystallographic sites: one is fully occupied cobalt (Co1) site and another one mixed site between antimony and selenium (Sb1/Se1). Electronic band structure of the compounds was studied using DFT calculations. The electrical transport properties such as electrical conductivity and thermopower analysis were carried out. Various thermal transport properties such as thermal diffusivity and specific heat capacity were studied. Finally the thermoelectric figure of merit was calculated and it was found 0.1 at room temperature and it increases as the temperature rises.

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