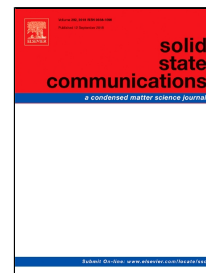


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Lattice dynamics, transport and superconducting properties of Ba-substituted Sr_3SnO

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Abstract

We have explored the lattice dynamics, transport and superconducting properties of Ba-substituted Sr_3SnO ($\text{Sr}_{3-x}\text{Ba}_x\text{SnO}$, $x=0, 1, 2$) using density functional theory (DFT) and density functional perturbation theory (DFPT). All the studied alloys show good dynamical stability. These Ba-substituted systems show metallic band structure due to the mixing of Sr-4d and Ba-5d with Sn-5p orbitals. According to Migdal-Eliashberg theory the calculated electron-phonon coupling constant and logarithmic-averaged phonon frequency for Sr_2BaSnO are $\lambda=0.24$ and $\omega_{\text{ln}}=124.55\text{K}$, respectively and the corresponding $T_c=0.6\text{ K}$ while it is 0.2 K for SrBa_2SnO . Our analysis reveals that phonon softening by Ba-substitution is responsible for superconductivity in these alloys.

Keywords: C. Structural stability; D. Lattice thermal conductivity; D. Electronic transport; D. Superconductivity

1. Introduction

Lattice dynamics of a solid have a great importance in analyzing different physical properties, such as the thermoelectric figure of merit (ZT) and phase stability of the solid [1,2]. Lattice thermal

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