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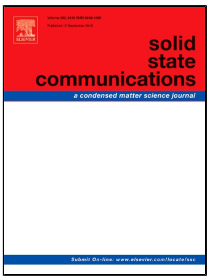

Lattice dynamics, transport and superconducting properties of Ba-substituted Sr_3SnO

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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 ($Sr_{3-x}Ba_xSnO$, 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 λ=0.24 and ω_{ln}=124.55K, respectively and the corresponding T_c=0.6 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