Electronic and thermoelectric properties of *p* type $CeFe_4Sb_{12}$

Nihal Limbu[1,2], Amit Shankar[2], and Atul Saxena[1]
[1]North-Eastern Hill University, Shillong, Meghalaya-793022.
[2]Condensed Matter Theory Research Lab, Kurseong college, Kurseong, 734203.

**Nihal Limbu: limbunihal08@gmail.com*

Abstract

The study of electronic and thermoelectric properties of $CeFe_4Sb_{12}$ was studied considering generalized gradient approximation (GGA) as exchange correlation functional using density functional theory. The sample material revealed the degenerate *p*-type semiconducting nature with an energy gap of 0.21 eV. The positive magnitude of Seebeck coefficient predicted holes to be the majority of charge carriers. The computed value of Seebeck coefficient at room temperature was found to be 79.1 μV/K, which is close to that experimental result. The nature of electrical conductivity suggested the degenerate behaviour of the sample alloy. The sample compound revealed lowest lattice thermal conductivity of 0.68 W/m-K with maximum *ZT* value of 0.53 at 800 K.

Introduction

Thermoelectric materials are the class of materials which convert industrial waste heat into usable electricity. The efficiency to convert heat into electricity is measured by the dimensionless figure of merit (*ZT*) of the material which is given by $ZT = S^2\sigma T/(K_e + K_L)$, where, *S* is Seebeck coefficient, σ is electrical conductivity, *T* is absolute temperature, K_e and K_L are electronic and lattice thermal conductivities respectively. Filled skutterudites [1] have emerged as potential thermoelectric material because of their excellent electrical conductivity and low lattice thermal conductivity. $CeFe_4Sb_{12}$ belongs to the class of thermoelectric material. Nouneh *et al.* revealed the semiconducting behaviour of $CeFe_4Sb_{12}$ with energy band gap of 0.66 eV [2] whereas Hachemou *et al.* displayed the energy band gap of 0.125 [3]. Experimental investigation reflected that the compound exhibited Seebeck coefficient of 79.4 μV/K at 300 K with maximum *ZT* value at 750 K [4].

In this manuscript, in order to tally the theoretical results with that experimental data, we have made an effort to analyse the electronic and thermoelectric properties of $CeFe_4Sb_{12}$ within generalised gradient approximation (GGA).

Computational details

The electronic properties of $CeFe_4Sb_{12}$ were explored using full potential linearized augmented plane wave (FP-LAPW) [5]. The exchange correlation interactions of the electrons were treated with GGA, For smooth band structure and transport properties calculations a grid of $10 \times 10 \times 10$ k points were considered. The energy convergence criterion was set to 10^{-6} Ry. The lattice thermal conductivity was calculated considering the Slack formalism [6]. And the thermoelectric properties were calculated using Boltztrap code [7].

Results and discussions

The energy band structures and the electronic density of states (DOS) are depicted in Fig. 1. The sample alloy reveals the semiconducting nature with top of valence band and minimum of conduction band occurring at Γ and Γ-*H* symmetry point respectively giving an indirect energy band gap of 0.21 eV. The valence band maximum at Γ point at the Fermi energy level (E_F) were found to be parabolic in nature (Fig. 1a) with an effective mass of $2.41m_e$ whereas the dense and flat bands just above E_F is observed which is contributed from the Ce-*f* electronic state as revealed by electronic density of states (Fig. 1b).

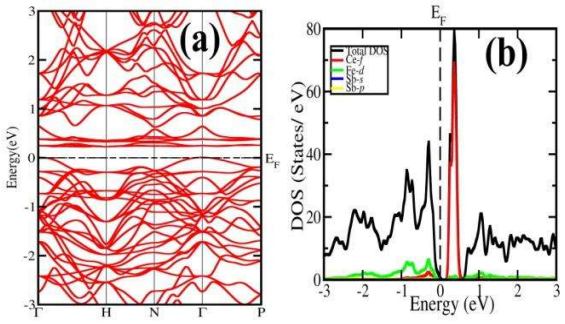

Fig. 1. Energy band structure (a) and density of states (b) of $CeFe_4Sb_{12}$.

The projected density of states predicted that the conduction region close to E_F was mainly dominated by Ce-*f* states whereas the valence region was populated by Fe-*d* states. Hybridization between