Materials Research Express

PAPER

Electronic structure, optical and thermoelectric properties of $CaMgSi_{1-x}C_x$ (x = 0, 0.5): an *ab-initio* study

RECEIVED
1 October 2018

REVISED
30 November 2018

ACCEPTED FOR PUBLICATION
11 December 2018

PUBLISHED
21 December 2018

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Keywords: electronic structure, thermoelectric properties, optical properties, seebeck coefficient, optical absorption

Abstract

In this study, the CaMgSi and its subsequent doping by carbon atoms has been systematically studied using the first-principles calculations. Ground state properties focusing particularly on the structural, optical and transport coefficients of these alloys are discussed. Semi-metallic character is prominent from the observed band profiles when GGA scheme is utilized. The enhancement of thermoelectric properties with a speculation from the electronic structure is observed when doped with carbon. Also, the thermoelectric properties are envisaged within the specific transport constraints in order to figure out the dimensionless figure of merit (zT). The Seebeck, electrical and thermal conductivity coefficients are calculated and thereby utilized to find out the extremum of zT for both these alloys. The maximum zT for CaMgSi is found to be 0.4 at 400 K and for CaMgSiC, its value increases to 0.8 at 800 K. Thus, the later compound can be developed as a high temperature thermoelectric material. The optical considerations of such alloys are predicted from the calculated values of optical conductivity, reflectivity and electron energy loss within the range of 30.00 eV of incident photons. Likewise, the active region of these alloys for possible application in optoelectronic devices is ultraviolet region because the ultraviolet frequencies are strongly absorbed by these compounds.

Introduction

Thermoelectric (TE) materials may contribute soon as new sources of ecofriendly and alternative to sustainable energy. Thermoelectric devices have found possible applications in electronic refrigeration, power generation, etc [1, 2]. Hence, the thermoelectricity could be an important parameter to discuss the possible solutions of persisting energy crisis. The efficiency of thermoelectric materials is guided by a well-known equation [3];

$$zT = S^2\sigma T/\kappa$$

Where zT is a dimensionless constant also known as figure of merit, S is the Seebeck coefficient, σ is the electrical conductivity, T is temperature and $\kappa = \kappa_L + \kappa_e$ is the total thermal conductivity which arises from two key parameters, i.e. the lattice part κ_L and the electronic part κ_e. For a TE material, the high performance could be achieved only if it exhibits high Seebeck coefficient, large electrical conductivity and low thermal conductivities. In a typical TE material, an in-detail understanding of electron-phonon transport interactions need be figured out for productive strategies to tailor these transport parameters [4, 5]. Improving the thermoelectric efficiency by altering the involved coefficients is one of the greatest challenges in materials science. As well as, the main objective in this area is to identify effective, low-cost and environmentally harmless solid thermoelectric