

Accepted Manuscript

Ternary germanide Li_2ZnGe : A new candidate for high temperature thermoelectrics

Saleem Yousuf, Dinesh C. Gupta



PII: S0925-8388(17)34407-9

DOI: [10.1016/j.jallcom.2017.12.211](https://doi.org/10.1016/j.jallcom.2017.12.211)

Reference: JALCOM 44297

To appear in: *Journal of Alloys and Compounds*

Received Date: 16 October 2017

Revised Date: 6 December 2017

Accepted Date: 19 December 2017

Please cite this article as: S. Yousuf, D.C. Gupta, Ternary germanide Li_2ZnGe : A new candidate for high temperature thermoelectrics, *Journal of Alloys and Compounds* (2018), doi: 10.1016/j.jallcom.2017.12.211.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Ternary Germanide Li₂ZnGe: A New Candidate for High Temperature Thermoelectrics

Saleem Yousuf and Dinesh C. Gupta*

Condensed Matter Theory Group, School of Studies in Physics

Jiwaji University, Gwalior – 474 011 (MP), INDIA

Email: sosfizix@gmail.com*; nengroosaleem17@gmail.com;

Abstract

Experimentally studied F-43m structured Li₂ZnGe ternary germanide is investigated theoretically by evaluating the electronic structure, thermodynamic stability and thermoelectric efficiency using the full-potential method. The calculated lattice parameter and structural characterization agree well with the experimental results. The thermoelectric properties are calculated within the temperature range of 0-1200 K. The computed value of figure of merit is 0.40 at 1200 K and Seebeck coefficient is 150 μ V/K specifying n-type nature. The electrical conductivity is high mainly due to high carrier mobility, while total thermal conductivity is moderate due to low lattice thermal conductivity. The estimated figure of merit projects it as a potential thermoelectric material for high temperature power generation.

Keywords: Ternary germanide; Electronic structure; Band structure; Thermoelectric properties; Thermodynamic properties.

I. Introduction

Applications of thermoelectric materials at cryogenic as well as thermogenic temperatures has given rise to considerable interest from the scientific community probably due to the severe exploitation of fossil fuels and an ever-increasing demand for a sustainable supply of energy [1-3]. They are envisaged with the ability to directly convert thermal and electrical energy to provide an alternative route for power generation and refrigeration. The factor establishing the efficiency of conversion is defined by dimensionless figure of merit (zT) [4-9]

$$zT = \frac{S^2 \sigma T}{\kappa_{\text{electronic}} + \kappa_{\text{lattice}}} \quad (1)$$

Download English Version:

<https://daneshyari.com/en/article/7994089>

Download Persian Version:

<https://daneshyari.com/article/7994089>

[Daneshyari.com](https://daneshyari.com)