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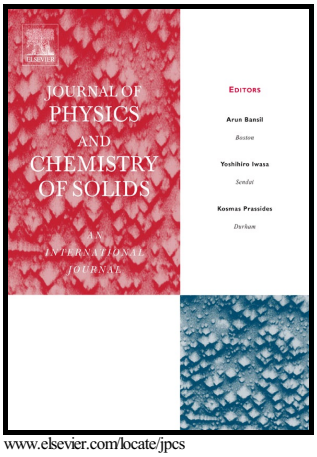


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Saleem Yousuf, Dinesh C. Gupta

PII: S0022-3697(16)31297-5
DOI: http://dx.doi.org/10.1016/j.jpcs.2017.04.023
Reference: PCS8050

To appear in: *Journal of Physical and Chemistry of Solids*

Received date: 15 December 2016
Revised date: 28 April 2017
Accepted date: 29 April 2017

Cite this article as: Saleem Yousuf and Dinesh C. Gupta, Temperature and Pressure Dependent Structural and Thermo-Physical Properties of Quaternary CoVTiAl Alloy, *Journal of Physical and Chemistry of Solids* http://dx.doi.org/10.1016/j.jpcs.2017.04.023

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# Temperature and Pressure Dependent Structural and Thermo-Physical Properties of Quaternary CoVTiAl Alloy

Saleem Yousuf, Dinesh C. Gupta*

Condensed Matter Theory Group, School of Studies in Physics Jiwaji University, Gwalior – 474 011 (MP), INDIA

*sosfizix@gmail.com

nengroosaleem17@gmail.com

## Abstract

Investigation of band structure and thermo-physical response of new quaternary CoVTiAl Heusler alloy within the frame work of density functional theory has been analyzed. 100% spin polarization with ferromagnetic stable ground state at the optimized lattice parameter of 6.01 Å is predicted for the compound. Slater-Pauling rule for the total magnetic moment of 3 $\mu_B$ and an indirect semiconducting behavior is also seen for the compound. In order to perfectly analyze the thermo-physical response, the lattice thermal conductivity and thermodynamic properties have been calculated. Thermal effects on some macroscopic properties of CoVTiAl are predicted using the quasi-harmonic Debye model, in which the lattice vibrations are taken into account. The variations of the lattice constant, volume expansion coefficient, heat capacities, and Debye temperature with pressure and temperature in the ranges of 0 GPa to 15 GPa and 0 K to 800 K have been obtained.

**Keywords:** DFT; Electronic structure; Mechanical properties; Thermoelectric properties; Thermodynamic properties

## Introduction

The alternate sources of energy in present scenario are thermoelectric (TE) [1-3] materials due to their ability to convert waste heat into electricity. TE materials could play an important role to build an efficient and sustainable energy portfolio. Efforts are underway to increase their efficiency, stability and cost for their potential practical applications. Harvesting of waste heat exhausts from various

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