PAPER

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IOP Publishing Semiconductor Science and Technology
Semicond. Sci. Technol. 32 (2017) 125019 (8pp) https://doi.org/10.1088/1361-6641/aa9785

DFT investigations on mechanical stability, electronic structure and magnetism in Co_2TaZ (Z = Al, Ga, In) heusler alloys

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Received 3 July 2017, revised 22 October 2017
Accepted for publication 1 November 2017
Published 22 November 2017

Abstract

Ferromagnetic Heusler compounds have vast and imminent applications for novel devices, smart materials thanks to density functional theory (DFT) based simulations, which have scored out a new approach to study these materials. We forecast the structural stability of Co_2TaZ alloys on the basis of total energy calculations and mechanical stability criteria. The elastic constants, robust spin-polarized ferromagnetism and electron densities in these half-metallic alloys are also discussed. The observed structural aspects calculated to predict the stability and equilibrium lattice parameters agree well with the experimental results. The elastic parameters like elastic constants, bulk, Young's and shear moduli, poison's and Pugh ratios, melting temperatures, etc have been put together to establish their mechanical properties. The elaborated electronic band structures along with indirect band gaps and spin polarization favour the application of these materials in spintronics and memory device technology.

Keywords: electronic structure, ferromagnetism, mechanical properties, half- metallicity, Heusler alloys

(Some figures may appear in colour only in the online journal)

1. Introduction

Ferromagnetic intermetallic alloys have been a subject of interest for researchers and industrialists throughout the globe due to the advancement in the fields of magnetoelectronics, memory device technology and spintronics e.g. spin transistors, magnetoresistive random access memories (MRAMs), spin valve generators, spin torque oscillators (STO) and read heads for hard disk drives (HDDs) [1–4]. Exhibition of spin polarization around the Fermi level, and ferromagnetic interaction along with large Curie temperature has intensified the interest in half-metallic materials, particularly the Heusler alloys [5, 6]. In half-metallic ferromagnets the coexistence of metallic electronic band profile in majority-spin and a minority-spin semiconducting electronic band structures are observed. Owing to this, the maximum efficiency of a spintronic device can be achieved due to production of spin polarized current from such materials [7–9]. Furthermore, an interesting rule called the Slater Pauling rule is followed by almost all these half-metallic Heusler alloys where the linear scaling of the total number of valence electrons in the unit cells is associated with the total spin magnetic moment [9]. Even though a vast collection of newly predicted half-metallic Heusler alloys have been added to this family, still novel properties are being discovered among them, which flag the way for diverse applications e.g. Spintronics/thermoelectrics/magnetoelectronics [10, 11]. For high temperature stability, Heusler alloys are the best candidates for shape memory devices and have a possible application in high temperature power generation [12, 13].

Transition metal based Heusler compounds have been extensively studied by researchers worldwide. Particularly, the Cobalt based Heusler compounds have attracted much interest due to the exhibition of large tunnel magneto-resistance (TMR), such as quaternary $Co_2Cr_{0.6}Fe_{0.4}Si$ [14]. Such phenomenon boosts the necessary investigations into Co-based Heusler

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