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Iridium's influence on the structural, electronic and mechanical characteristics of $ZrCo_{1-x}Ir_xSb$ half-heusler alloys

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ABSTRACT

Structural, electronic and mechanical *properties of* $ZrCo_{1-x}Ir_xSb$ *Half-Heusler alloys with varying x concentrations (x = 0, 0.125, 0.25, 0.375, 0.5, 0.625, 0.75, 0.875, and 1) were studied by performing the exchange-correlation (XC) energy evaluated using the local density (LDA) and generalized gradient (GGA) approximations. The calculated lattice constant, bulk modulus, and band gap energy of the ternary alloy show good agreement with previous theoretical predictions. The results indicate that an increase in Ir atom concentration in the alloy leads to an enlargement of the lattice constant (from 6.10 to 6.36 Å) and bulk modulus (from 138.09 to 149.70 GPa), resulting in increased volume and hardness of the compound. Moreover, the Engel-Vosko generalized gradient approximation (EVGGA) and modified Becke-Johnson (mBJ) schemes were employed to improve the calculations of the band structure and density of states. The studied alloys exhibit semiconductor characteristics, with a direct band gap for both x = 0.75 and x = 0.875 concentrations and an indirect band gap for the rest of the concentrations.* The computed elastic constants for $ZrCo_{1-x}Ir_xSb$ alloys satisfy the requirements for mechanical stability. The VRH approximations have been used to determine the bulk modulus, shear modulus, Young's modulus, Poisson's ratio and Hardness. In addition, we also determined the anisotropy factor, sound velocities and Debye temperature.

1. Introduction

Heusler alloys, named after Fritz Heusler, the German metallurgical engineer and chemist who discovered them in 1903 while he was studying the electrical conductivity of certain metallic alloys. He observed that an alloy composed of copper, manganese, and aluminum (Cu_2MnAl) displayed ferromagnetic properties, even though none of its constituent elements were magnetic on their own [1–18]. This unexpected behavior intrigued researchers and led to further exploration of this new class of materials.

Heusler alloys are an amazing group of materials, and there are thousands of them today. Our study focuses on a particular type called "Half-Heusler" alloys, not "Full-Heusler" alloys. The special thing about Half-Heusler alloys is that they have relatively high Curie temperatures [19–22] and their structure is similar to the zinc blende phase. This similarity allows for the possibility of integrating magnetic devices into semiconductor technologies.

The compounds known as half-Heusler (HH) alloys have a structure called MgAgAs [23]. XYZ, an HH alloy, has a structure that is similar to the structure of a full-Heusler alloy X_2YZ. In this structure, X and Y are transition metals, and Z is an element from group III, IV, or V on the periodic table. However, sometimes Y is replaced by a rare earth or alkaline earth metal element. Fig. 1 illustrates the displayed structure. This type of half-Heusler structure is characterized by three interpenetrating sub-lattices of a face-centered cubic arrangement, with each lattice occupied by atoms X, Y, and Z [24]. Wyckoff's notations are used to describe the locations of atoms, such as 4a (0, 0, 0), 4b (1/2, 1/2, 1/2), and 4c (1/4, 1/4, 1/4) [25–27]. In theory, there are three different possible atomic arrangements in this type of structure, as shown in Table 1.

Half-Heusler alloys are known for their ability to combine with various elements. This combination leads to a diverse set of physical properties. Heusler alloys are fascinating materials that exhibit a range of unique properties, including ferromagnetism, shape memory, and

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