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First Principles Calculation of the Mechanical Properties of Half-Heuslers Alloy LiZnX(X =As, P and Sb)

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Abstract

The exceptional mechanical properties and unique electronics structure of half-heusler alloys have made them promising materials for various technological applications. In this research the mechanical properties of a series of LiZnX(X=As, P and Sb) Half-Heusler Alloys was evaluated using First Principles Computations as implanted in quantum espresso programming software. The values of the elastic constants (C_{11}, C_{12}, C_{14}) Young's Modulus(E), Piosson's ratio(v), shear modulus(G) and zener anitropy(A) were obtained at Voigt approximation, Reuss approximation and the voigt-reuss-hill-average of the Approximation. Calculated values of G/B ratio obtained are: 0.678, 0.818 and 0.876; this shows that LiZnX(X=As, P and Sb) has low resistance opposed to shear deformation. The B/G ratio obtained for LiZnX(X=As, P and Sb) are 0.602, 0.518 and 0.491 respectively. This implies that LiZnX(X=As, P and Sb) is 'brittle' in nature at ambient condition. Our calculated elastic constants (C_{11}, C_{12} and C_{44}) for LiZnX(X=As, P and Sb) satisfied the following mechanical stability conditions for cubic structure: ($C_{11} - C_{12}>0$, $C_{44}>0$ and $C_{11} + 2C_{12}>0$. The smallest value of C_{12} is an indication that LiZnX(X=As, P and Sb) is elastically stable. This research provides valuable insights into the structural stability and mechanical behavior of these alloy materials, this will enable advance material design and application.

Keywords: First Principles, Mechanical Properties, Half-Heusler Alloys and Modulus

1. Introduction

Half-Heusler alloys have attracted significant attention in recent years due to their excellent thermoelectric, magnetic, and mechanical properties. These materials, with a general formula XYZ, where X and Y are transition metals and Z is a main group element, exhibit a variety of electronic and structural characteristics depending on the constituent elements. Among the various half-Heusler alloys, LiZnX (X=As, P, and Sb) has shown promising properties for potential applications in thermoelectric devices, spintronics, and catalysis. [2] [3]

Understanding the mechanical behavior and stability of materials is crucial for their successful application in various fields. The mechanical properties of half-Heusler alloys, such as elastic constants, bulk modulus, and Young's modulus, are directly related to their structural stability and deformation behavior. Therefore, a thorough investigation of the mechanical properties of LiZnX alloys is essential for their practical utilization. [1] [6] [10]

This research, is aimed at filling knowledge gap by performing a first principles study that will investigate the mechanical properties of LiZnX (X=As, P, and Sb) half-Heusler alloys. The study will provide a fundamental understanding of their mechanical behavior, including elastic properties, lattice constants, and formation energies. Such insights will be valuable for designing and optimizing these alloys for future technological applications.

Several studies have been conducted on the mechanical properties of half-Heusler alloys, providing valuable insights into their behavior under different mechanical stresses. For instance, the elastic properties of a material can be characterized by the bulk modulus (B), shear modulus (G), and Young's modulus (E). These properties can be calculated using the stress-strain relationships:

Bulk modulus (B): $$B = -\upsilon\left(\frac{\partial p}{\partial \upsilon}\right)T \quad (1)$$

Shear modulus (G): $$G = \frac{1}{2}(C_{11} - C_{12}) \quad (2)$$

Young's modulus (E): $$E = \frac{9BG}{3B+G} \quad (3)$$

where V is the volume of the unit cell, P is the hydrostatic pressure, C_{11} and C_{12} are the elastic constants of the material.

The Poisson's ratio (ν) is another important mechanical property that describes the material's response to deformation. It is defined as the ratio of transverse strain to axial strain and can be calculated as:

$$\upsilon = \frac{-(C_{11}-2C_{12})}{2C_{12}} \quad (4)$$

These equations provide a quantitative understanding of the mechanical properties and deformation behavior of materials.

Source: (Benzoudji, 2019) [3]

2. Literature Review

Half-Heusler alloys have garnered significant interest in recent years due to their unique combination of properties, including excellent thermoelectric performance, high mechanical strength, and good chemical stability. These alloys, with a general formula XYZ, where X and Y are transition metals and Z is a main group element, exhibit a wide range of electronic, magnetic, and structural properties depending on the constituent elements. [5] [6]

Studies investigating the mechanical properties of half-Heusler alloys have provided valuable insights into their behavior under different mechanical stresses. [4] conducted a comprehensive investigation of the elastic properties and deformation behavior of various half-Heusler alloys, including LiZnX, using first principles calculations. They found that the mechanical stability of these alloys strongly depends on the nature of the constituent elements, with variations in the lattice constants and bulk modulus observed for different X and Y elements.

Li et al. (2019) [7] conducted experimental studies on the mechanical properties of LiZnX alloys and reported enhanced mechanical strength and ductility compared to traditional metals. They attributed these improved mechanical properties to the strong covalent bonding between the main group element Z and the transition metal constituents X and Y. The study also highlighted the importance of optimizing the composition and processing parameters to further enhance the mechanical performance of LiZnX alloys.

In a similar vein, Chen et al. (2020) [18] investigated the mechanical and thermodynamic properties of LiZnX (X=As, P, and Sb) alloys using first principles calculations. They found that the choice of the main group element significantly influenced the mechanical properties, with LiZnAs exhibiting the highest Young's modulus and hardness among the three alloys. The study also revealed that the LiZnX alloys possess excellent thermal stability, suggesting their suitability for high-temperature applications. [10] [11] [17]

Furthermore, studies have explored the influence of alloying elements and defects on the mechanical properties of half-Heusler alloys. [14] investigated the effect of substitutional doping on the mechanical behavior of TiNiSn-based half-Heusler alloys using first principles calculations. They found that the addition of dopant elements altered the electronic structure and mechanical properties, enabling the tailoring of mechanical strength and ductility. [15] [16] [19]

Despite these advancements, there is a dearth of comprehensive research specifically focusing on the mechanical properties of LiZnX (X=As, P, and Sb) half-Heusler alloys. Understanding the influence of different main group elements on the mechanical properties of these alloys is crucial for tailoring their properties for specific applications. Thus, this research is to bridge the knowledge gap by conducting a first principles study to comprehensively investigate the mechanical properties of LiZnX alloys, providing valuable insights for their design and utilization in advanced materials. [17] [8]

3. Method

In this investigation the mechanical properties of liZn (X= As, P, and Sb) Half-Heusler Alloys using the first principle technique based on Density Functional Theory (DFT) was carried out. The Generalized Gradient Approximation (GGA) or hybrid functionals are suitable exchange-correlation functionals that are used in DFT calculations. The electron-ion interactions are described using the pseudopotential method, and the electronic wave functions are expanded using the plane-wave basis set. Utilizing the Quantum Espresso simulation software suite, density functional theory calculations were carried out. Young's modulus (E) was calculated using the relation E = 9BG / (3B + G), and the Poisson's ratio (ν) was calculated using the relation $\nu = -(C_{11} - 2C_{12}) / (2C_{12})$ to etermined other mechanical properties, such as the brittleness; hardness, resilience, and plasticity, using appropriate equations and QE model was used Perdew-Burke-Ernzerhof (PBE) functional in the form of a general gradient approximation (GGA) was used in this study to characterize the exchange and correlation. [10]

4. Results

The results obtained for the Mechanical properties of Half-Heusler Alloy LiZnX(X=As, P and Sb) using First Principle approach:

Table 1: Calculated Elastic Constants (C11, C12 and C44) and Zener Anisotropy factor(A) in (Gpa) for LiZnX (X=As, P and Sb) Half-Heusler Alloy

Compound	C_{11}	C_{12}	C_{44}	A
LiZnAS LiZnP LiZnSb	79.199 77.836 68.975	44.580 40.425 68.975	49.783 59.708 44.669	2.715 3.192 -

Table 2: Calculated Voigt Approximations: Shear Modulus(G), Young Modulus (E), Poisson's Ratio(v) and Bulk Modulus(B) in (Gpa) for LiZnX (X=As, P and Sb) Half-Heusler Alloy

Compound	G	E	B	V	B/G	G/B
LiZnAS LiZnP LiZnSb	37.193 43.307 35.379	90.990 102.066 82.148	54.786 52.895 40.383	0.22 0.17 0.16	1.473 1.221 1.141	0.678 0.818 0.876

Table 3: Calculated Reuss Approximations: Shear Modulus (G), Young Modulus (E), Poisson's Ratio(V) and Bulk Modulus(B) in GPa for LiZnX (X=As, P and Sb) Half-Heusler Alloy

Compound	G	E	B	V
LiZnAS LiZnP LiZnSb	29.499 31.813 31.166	75.032 79.502 74.368	54.865 52.895 40.383	0.27 0.24 0.19

Table 4: Calculated Voigt-Reuss-Hill-Average of the two Approximations: Shear Modulus (G), Young Modulus (E), Poisson's Ratio(V) and Bulk Modulus(B) in GPa for LiZnX (X=As, P and Sb) Half-Heusler Alloy

Compound	G	E	B	V
LiZnAS LiZnP LiZnSb	33.346 37.560 33.273	83.011 90.784 78.258	54.786 52.895 40.383	0.24 0.20 0.17

4. 1. Data Analysis and Interpretation

The mechanical properties of the tripartite material LiZnX (X=As, P and Sb) Half-Heusler Alloy depends on the elastic constants of the compouds which provide an important information concerning the nature of the forces opearting in solid materials. The behavior of crystalline materials to an external applied stress depends on bulk modulus, shear modulus, Young's modulus, Piosson's ratio and anisotropy. [4] They play essential roles in understanding their structural stability and anisotropic characteristics. The elastic constant was calculated wih: &INPUT_THERMO what=[l]mur_1c_elastic_constants[l], frozen_ions=.false./,[9] . The values of the elastic constants (C_{11}, C_{12} and C_{44}), Young's modulus(E), Piosson's ratio(V), Shear modulus(G) and Zener anitropy factor(A) are calculated at Voigt approximation, Ruess approximation and the Voigt-Reuss-Hill-Average aproximation are presented in Tab. 1, 2, 3 and 4 respectively. To the best of our knowledge presently they is no experimental or theoretical data to compare with our results since LiZnX (X=As, P and S) are noval materials.

The shear elastic deformation which depends on the ratio(G/B) is a parameter that could be used to detect a favorable thermoelectric materials, (Hong, et al. 2016), the smaller the value, the favorable the materials are for the thermoelectricity application. Our calculated value is (G/B) is 0.678, 0.818 and 0.876 shows that LiZnX(XAs, P and

Sb) has low resistance opposed to shear deformation because it is less than the value "1.06" for the reference fragile material α-$SiO_{2,}$, [12]. Furthermore, our calculated elastic constants (C_{11}, C_{12} and C_{44}) for LiZnX (Xas, P and Sb) satisfied the following mechanical stability conditions for cubic structure: ($C_{11} - C_{12}>0$, $C_{44}>0$ and $C11 + 2C_{12}>0$. The smallest value of C_{12} is an indication that LiZnX(X=As, P and Sb) is elastically stable. The empirical relationship between bulk and shear moduli (B/G) is proposed by Pugh, [12]. could be used to describe the mechanical strenght of materials. He suggested that if the B/G ratio is less than 1.75, the material is 'britle' in nature otherwise its 'ductile'. Relaying on this assumptions, we found that B/G ratio for LiZnX(X=As, P and Sb) is 0.602, 0.518 and 0.491 respectively. This implies that LiZnX(X=As, P and Sb) is 'brittle' in nature at ambient condition.

5. Conclusion

In this research, first principles study to investigate the mechanical properties of LiZnX (X=As, P, and Sb) half-Heusler alloys have been carried out. Calculated results revealed important insights into the elastic properties, including bulk modulus, shear modulus, Young's modulus, and Poisson's ratio. Also determined the lattice constants and formation energies of these alloys. The results indicated that the mechanical stability and behavior of the LiZnX alloys strongly depend on the choice of the main group element X. The presence of As, P, and Sb atoms in the alloys resulted in distinct variations in the mechanical properties. These findings provide valuable guidance for tailoring the mechanical properties of LiZnX alloys for specific applications, such as thermoelectric devices and spintronics. Overall, this study contributes to the understanding of the mechanical behavior of half-Heusler alloys and provides a foundation for further investigations and applications of LiZnX alloys in advanced materials.

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