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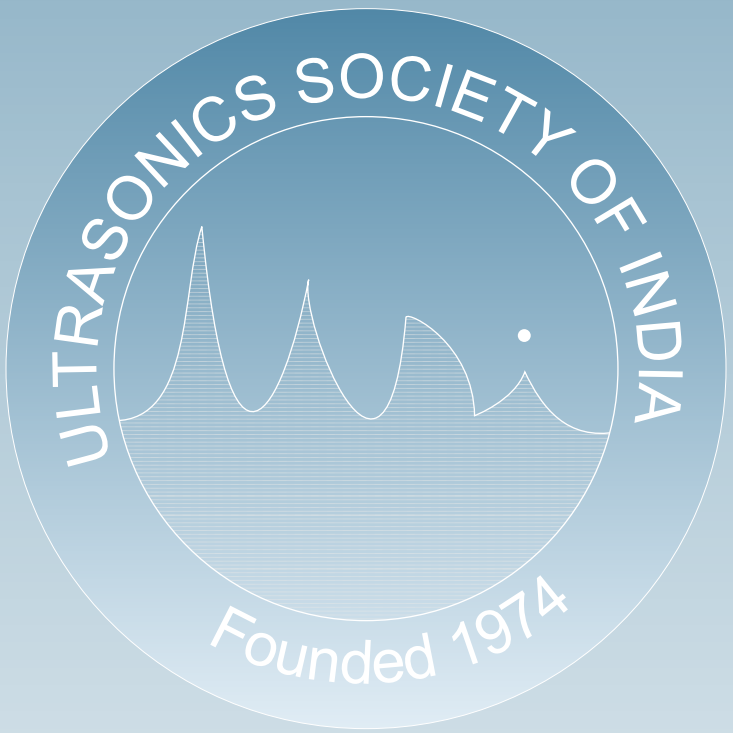

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CONTENTS

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Study of mechanical properties of β Phase Zr-Ti-X Alloys (X= Al, V)

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In this work, we have used the Interaction potential model to study the mechanical characteristics of Zr-Ti-X alloys in the β phase (where X = Al, V). The mechanical properties of Zr-Ti-X alloys show promise in the β phase, and an understanding of its behavior at the atomic level can yield important insights for real-world applications. This study aims to investigate mechanical properties, including bulk modulus, shear modulus, Young's modulus, and elastic constants. The mechanical behavior of the β phase is known to be influenced by the alloying elements Al and V. Therefore, it is important to comprehend their impacts in order to create alloys with certain qualities. Here, we've looked at how ductility reduces with increasing mass fractions of Al in Zr-Ti-Al alloys and increases with mass fractions of V in Zr-Ti-V alloys.

Keywords: Mechanical properties, Poisson's ratio, elastic constants.

Introduction

The mechanical properties of body-centered cubic (BCC) alloys are influenced by various factors such as microstructure, phase composition, and alloying elements. High-entropy alloys' microstructure and mechanical characteristics have been demonstrated to be greatly impacted by annealing processes, with the precipitation of BCC phases affecting their characteristics[1]. Because of the creation of disordered BCC matrices and embedded precipitates, the inclusion of elements such as Al can result in the generation of alloys with desired mechanical characteristics[2]. Phase stability, microstructural characteristics, alloy composition, and other factors all affect the mechanical properties of β phase Zr-Ti-X alloys. Research on Zr-Ti-X alloys with various alloying components has revealed important effects on the mechanical characteristics. For example, studies have been conducted to determine the impact of Ti addition on the mechanical characteristics and structure of Zr-Ta alloys[3]. Zr-Ti-X alloys' mechanical characteristics can be customized by adjusting the phase composition and structure. Studies on Zr-Ti-X alloys including Al and V have shown that phase compositions and structures have a major effect on the alloys' mechanical properties.The significance of Zr and Ti content in influencing the mechanical properties of multiphase Zr alloys has been emphasized by studies on Zr-Ti-Al and Zr-Ti-V compositions[4]. Ultrasonic technique has been thoroughly investigated for several uses, such as the creation of bulk glassy alloys with excellent ductility and strength[5]. It has been discovered that adding Zr to Ni-Ti-Al alloys affects their mechanical characteristics and microstructures, causing new phases and solid solution components to develop[6]. Ti-Zr alloys have demonstrated encouraging outcomes in the field of biocompatibility. These alloys have much superior mechanical qualities when compared to pure metals[7]. At room temperature superelasticity has been studied for Ti-Mo-Sn-Zr alloys, and several of these alloys exhibit good superelastic behavior[8]. The existence of distinct phases affects the microstructure and characteristics of these alloys. According to studies, Zr can stabilize the phase in Ti-based alloys. For example, Zr can prevent the formation of an intermetallic phase in Ti-Ni-Cu-Sn-Zr alloys that resembles a complicated solid solution[9]. it has been discovered that Zr addition to Ti-Mo-Sn alloys stabilizes the phase and influences the martensitic transformation temperature[10]. Zr has been demonstrated to improve the β phase stability in Ti-based shape memory alloys[11].

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To sum up, the study conducted on Zr-Ti-X alloys emphasizes the significance of alloying elements such as Nb, Al, V, and Zr in affecting the microstructure, phase stability, and characteristics of these alloys. Comprehending the function of these constituents is vital in customizing the properties of β-phase Zr-Ti-X alloys for diverse uses.

In this work, we investigated the relationship between Zr-Ti-X (X= Al, V) alloys' element composition using the interaction potential model. The atomic fraction of Al and V increases from 0 to 15at% in order to examine how alloying elements Al and V affect the mechanical properties of Zr-Ti-Al and Zr-Ti-V alloy systems.

Theory

Higher-order elastic constants : Higher-order elastic constants (HOECs) have been calculated in the current work using the interaction potential technique. The elastic energy density with strain can be estimated to get the higher-order elastic constants. The following equations can be used to mathematically express this[12]:

$$C_{ijklmn.....} = \left(\frac{\partial^n F}{\partial \eta_{ij} \partial \eta_{kl} \partial \eta_{mn.....}} \right) \quad (1)$$

Where η_{ij} represents the Lagrangian strain component and F represents free energy density.

F can be expended in terms of η

$$F = \sum_{n=0}^{\infty} F_n = \sum_{n=0}^{\infty} \frac{1}{n!} (\partial^n F / \partial_{\eta ij} \partial_{\eta kl} \partial_{\eta mn....}) \eta_{ij} \eta_{kl} \eta_{mn} \quad (2)$$

$$F = F_2 + F_3 \quad (3)$$

Where $F_2 = \frac{2}{2!} C_{ijkl} \eta_{ij} \eta_{kl}$, $F_3 = \frac{1}{3!} C_{ijklmn} \eta_{ij} \eta_{kl} \eta_{mn}$ (4)

Here C_{ij} are second-order elastic constants and C_{ijk} are third-order elastic constants. Second and third-order elastic constants can be written as[12-14]:

$$\begin{aligned}
C_{11}^0 &= \frac{3}{8}\frac{e^2}{r_0^4} S_5^{(2)} + \frac{3\phi(r_1)}{b_{ro}}\left(\frac{\sqrt{3}}{3_{r0}} + \frac{1}{b}\right) + \frac{2\phi(r_2)}{b_{ro}}\left(\frac{1}{2_{r0}} + \frac{1}{b}\right) \\
C_{12}^0 &= C_{44}^0 = \frac{3}{8}\frac{e^2}{r_0^4} S_5^{(1,1)} + \frac{\phi(r_2)}{b_{ro}}\left(\frac{1}{2_{r0}} + \frac{1}{b}\right) \\
C_{111}^0 &= \frac{15}{8}\frac{e^2}{r_0^4} S_7^{(3)} + \frac{\phi(r_1)}{9b}\left(\frac{\sqrt{3}}{r_0^2} + \frac{3}{b_{ro}} + \frac{\sqrt{3}}{b^2}\right) + \frac{\phi(r_2)}{2b}\left(\frac{3}{r_0^2} + \frac{6}{br_0} + \frac{4}{b^2}\right) \\
C_{112}^0 &= C_{166}^0 = -\frac{15}{8}\frac{e^2}{r_0^4} S_7^{(1,1)} - \frac{\phi(r_1)}{9b}\left(\frac{\sqrt{3}}{r_0^2} + \frac{3}{br_0} + \frac{\sqrt{3}}{b^2}\right) \\
C_{123}^0 &= C_{456}^0 = C_{144}^0 = -\frac{15}{8}\frac{e^2}{r_0^4} S_7^{(1,1,1)} - \frac{\phi(r_1)}{9b}\left(\frac{\sqrt{3}}{r_0^2} + \frac{3}{b_{ro}} + \frac{\sqrt{3}}{b^2}\right)
\end{aligned} \quad (5)$$

Where $\phi(r_1) = A \exp(-r_1 / b)$, $r_2 = 2r_0$ (6)

S is the lattice sum. The values of lattice sums are:

$$\begin{aligned}
&S_1^0 = -Z_0 = -1.017678,\ S_5^{(2)} = 0.354190,\ S_5^{(1,1)} = 0.346708 \\
&S_7^{(3)} = 0.540901,\ S_7^{(2,1)} = -0.093356,\ S_7^{(1,1,1)} = -0.159996
\end{aligned} \quad (7)$$

The value of A can be obtained with the equilibrium condition and is given as:

$$A = (bZ_0 e^2 / r_0^2)[8\sqrt{3} \exp(-r_1 / b) + 12 \exp(-r_2 / b)] \quad (8)$$

Mechanical Properties : Mechanical characteristics are evaluated to analyze the stability, microhardness, strength, and nature of the Zr-Ti-Al and Zr-Ti-V alloys with increasing atomic fraction (Al,V) from 0 to 15at%. We have calculated the alloy's bulk modulus, shear modulus, Young's modulus, and Poisson's ratio using the Voigt-Reuss-Hill technique[15]. The following equations can be used to calculate these physical quantities.

$$\begin{aligned}
&B_V = B_R = \frac{C_{11} + 2C_{12}}{3},\ B = \frac{B_V + B_R}{2},\ Y = \frac{9GB}{G + 3B}, \\
&G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5},\ G_R = \frac{5[C_{11} - C_{12}) C_{44}}{4[C_{44} + 3(C_{11} - C_{12})]}, \\
&G = \frac{G_V + G_R}{2},\ \sigma = \frac{3B - 2G}{6B + 2G}
\end{aligned} \quad (9)$$

Results and Discussion

Second-order elastic constants for β-phase Zr-Ti-Al and Zr-Ti-V alloys system calculated by the interaction model satisfied stability criteria[16,17]

$$\begin{aligned}
C_{11} + 2C_{12} &> 0 \\
C_{11} &> C_{12} \\
C_{44} &> 0
\end{aligned} \quad (10)$$

i.e. chosen alloys are stable. Fig. 1 tells the effect of Al and V atomic fractions on the independent elastic constants of the BCC-structured Zr-Ti-Al and Zr-Ti-V alloy systems.

From fig. 1 we found that the value of C_{11} is higher than other elastic constants. This implies that when subjected to uniaxial tension along its axis, is extremely incompressible.

A material's resistance to uniaxial pressures is measured by its Young's modulus, which serves as a stiffness indicator. Parallel to this, the bulk and shear modulus function as markers of resistance to changes in shape brought about by pressure and shear stress,

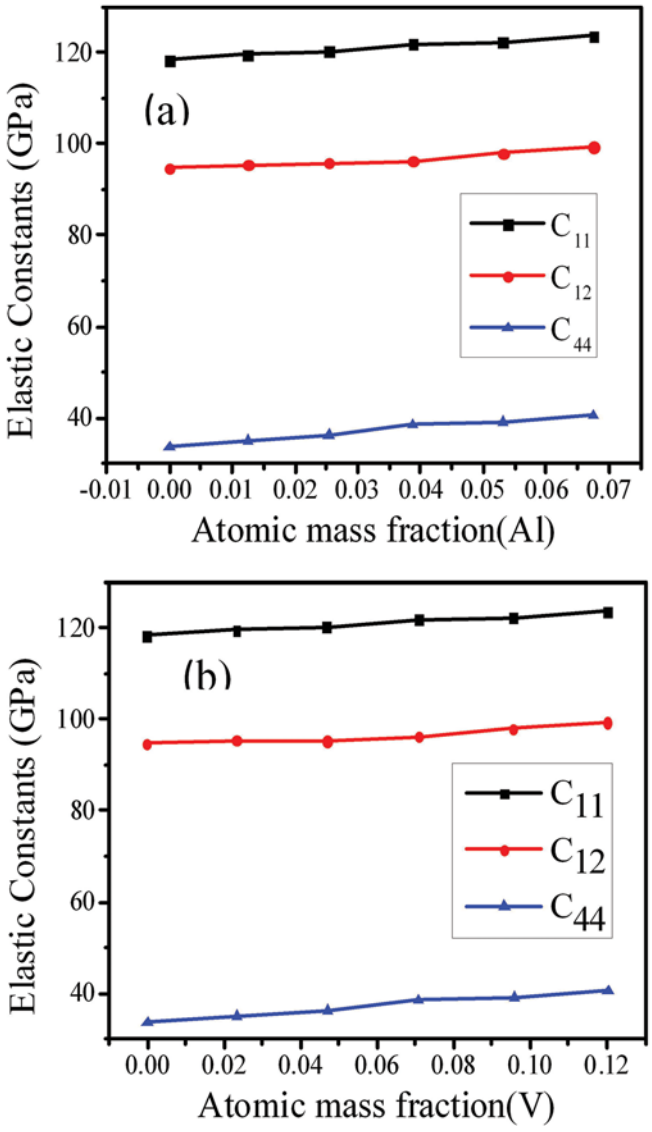

Fig. 1. Effect of Al atomic fraction (a) and V atomic fraction (b) on the elastic constants of β phase Zr-Ti-Al and Zr-Ti-V alloy systems.

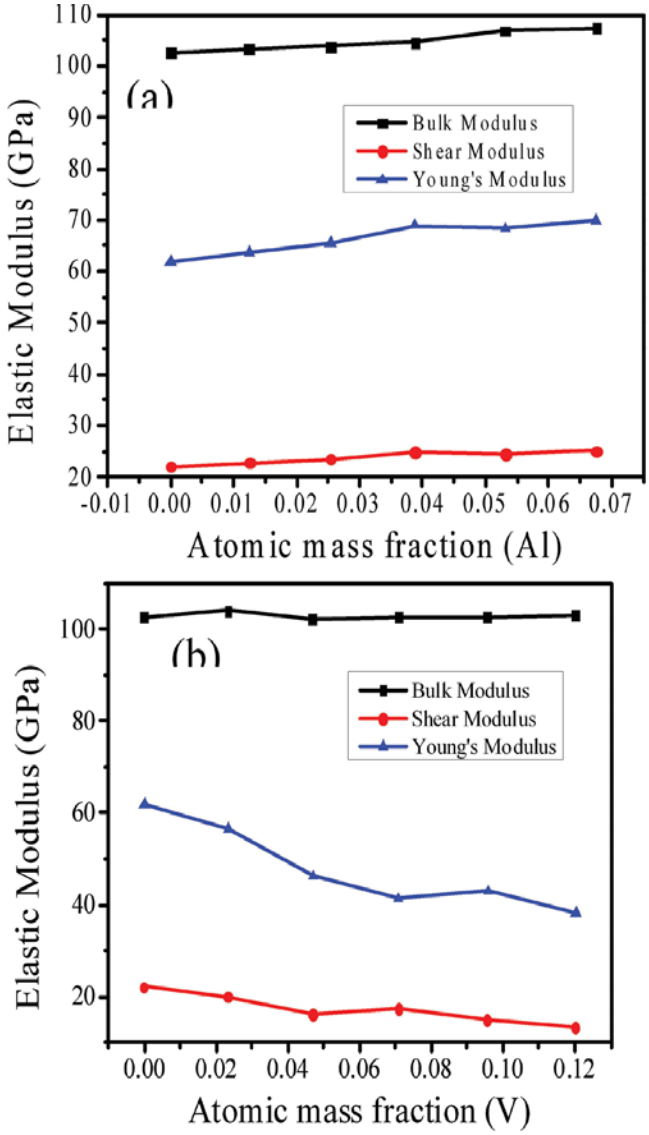

Fig. 2. Effect of Al atomic fraction (a) and V atomic fraction (b) on the elastic moduli of β phase Zr-Ti-Al and Zr-Ti-V alloys system.

respectively. The brittleness and ductility of the material are shown by the Poisson's ratio.

Fig. 2 illustrates the impact on elastic moduli by increasing the mass fractions of Al and V in the Zr-Ti-Al and Zr-Ti-V alloy systems.

From fig. 2 it is clear that the strength, hardness, and stiffness of Zr-Ti-Al increase as the mass fraction of Al increases. On the other hand as the mass fraction of V increases, the strength of the Zr-Ti-V alloy system increases but the hardness and stiffness of the alloys decrease.

Fig. 3 gives information about Poisson's ratio and mass fractions of Al and V in the Zr-Ti-X (X= Al,V) alloy system.

As found in fig. 3, in the Zr-Ti-X alloy system, the ductility of the Zr-Ti-Al alloy system decreases with an increase in the atomic fraction of Al, and the ductility of the Zr-Ti-V alloy system increases with an increase in the atomic fraction of V from 0 to 12 at%.

This means mechanical properties change due to changes in mass fraction for different compositions of Zr- Ti-X (X = Al, V) alloy systems.

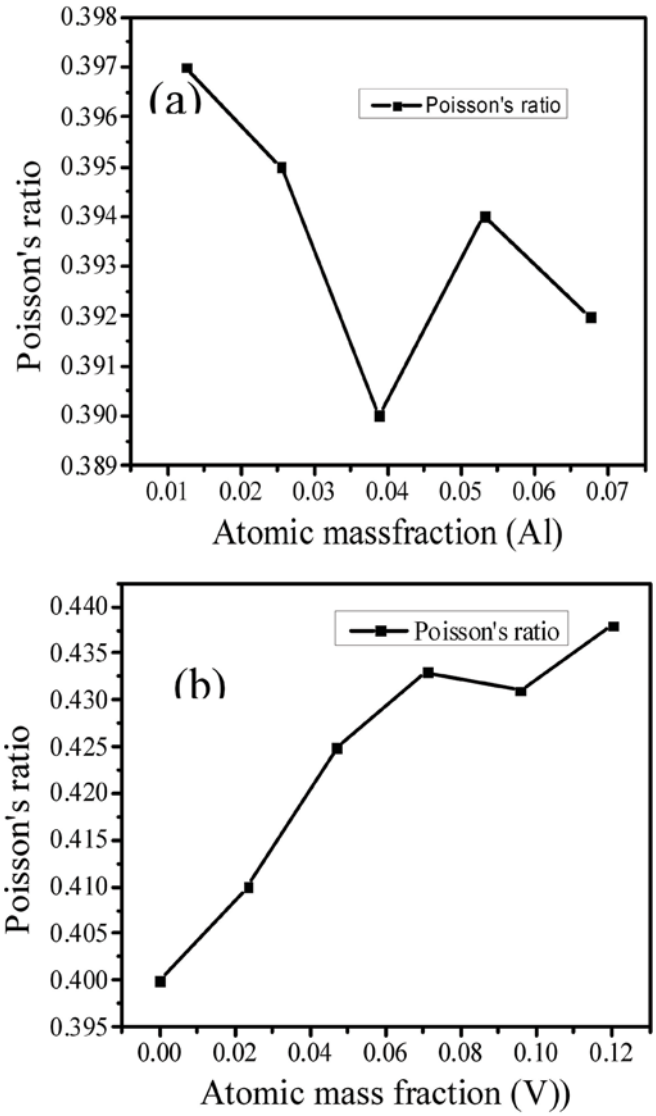

Fig. 3. Effect of Al atomic fraction (a) and V atomic fraction (b) on the Poisson's ratio of β phase Zr-Ti-Al and Zr-Ti-V alloys system.

Conclusion

In Zr-Ti-Al and Zr-Ti-V systems, the mass fraction of alloying elements has a major effect on the alloy's mechanical characteristics. V acts as a stabilizer for the Zr-Ti-V alloy system. This study indicates that in Zr-Ti-V alloys, the mass fraction of V significantly impacts the alloy's strength, hardness, and ductility. Zr-Ti-V alloys are more ductile than Zr-Ti-Al alloys with a change in atomic fraction from 0 to 15 at%. This suggests a complex interplay between alloy composition and mechanical properties. In conclusion, the strength, hardness, ductility, and corrosion resistance of the resulting materials can be precisely tailored by carefully modifying the mix of alloying elements in Zr-Ti-Al and Zr-Ti-V systems.

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