

Elastic Properties of As-Solidified Ti-Zr Binary Alloys for Biomedical Applications

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Young's modulus (E), shear modulus (G), bulk modulus (K) and Poisson's ratio (ν) of Ti-Zr binary alloys containing 20, 40, 50, 60, 70 and 80 at% Zr and component pure metals (Ti, Zr) prepared by arc-melting followed by solidification process were determined precisely by ultrasonic sound velocity measurements. X-ray diffraction analysis showed that all the as-solidified alloys and pure metals were with a single-phase structure of the hexagonal close-packed lattice (martensitically formed α' -phase). The alloying addition of Zr to Ti effectively decreased both E and G values with their minimum values of 89.5 ± 1.0 GPa and 33.3 ± 0.4 GPa, respectively, being recorded at the same composition Ti-60 at% Zr. On the other hand, K values decreased slightly when the concentration of Zr was increased from 20 to nearly 50 at% and further increases in Zr concentration did not change K values greatly. The observed variations of Young's modulus with Zr concentration in the entire range of composition were well interpreted in terms of density (ρ), Debye temperature (θ_D) and concentration of atoms (n) in each alloy. The quantity $\rho\theta_D^2 n^{-2/3}$ was revealed to be a good measure in predicting the tendency of variations of Young's modulus with composition in this binary system. [doi:10.2320/matertrans.MI201501]

(Received January 19, 2016; Accepted April 1, 2016; Published June 17, 2016)

Keywords: titanium-zirconium alloy, elastic property, Young's modulus, shear modulus, bulk modulus, ultrasonic sound velocity

1. Introduction

Titanium (Ti) and its alloys are attracting much attention in orthopedics because of their low density, high strength-to-density ratio, excellent biocompatibility and corrosion resistance. These superior qualities are advantageous for their application to various load-bearing artificial devices in a living body. Recently, various Ti alloys with low elastic moduli for biomedical applications are under development. Most of them are Ti-Al-, Ti-Mo-, or Ti-Nb-based multicomponent alloys consisting of three or more elements.¹⁾ Considering the fact that zirconium (Zr) is often added to these Ti alloys with low elastic moduli, Zr is implied to have a significant effect on lowering elastic moduli of Ti alloys.

The element Zr belongs to the group 4 in the periodic table, the same group as Ti, and is known to possess chemical properties and biocompatibility similar to that of Ti.^{2–4)} From the metallurgical aspects, the alloying addition of Zr to Ti gives rise to several advantages in producing load-bearing metallic biomaterials. First, the density of Zr has been reported to be 6.50 g cm^{-3} at 20°C ,⁵⁾ and this low density is favorable to fabricate light-weight Ti-Zr-based biomedical appliances. Second, Ti and Zr mix well together and the Ti-Zr binary system forms a continuous solid solution for both high temperature β -phase with the body-centered cubic (BCC) structure and low temperature α -phase with the hexagonal close-packed (HCP) structure throughout the entire range of composition.⁶⁾ From the viewpoint of chemical stability, this character of forming a single-phase structure at any composition is advantageous in preventing the galvanic corrosion in a body fluid compared with multi-phase alloys.^{7,8)} Third, the addition of Zr to Ti effectively lowers liquidus temperatures and the congruent temperature of 1540°C is attained at around Ti-38 at% Zr composition.⁶⁾ This effect of Zr addition on

lowering liquidus temperatures is advantageous in fabricating biomedical and other various industrial appliances by solidification process.

Since the load-bearing metallic biomaterials are used under the loading condition within their elastic limits in a living body, it is desirable that their elastic properties are as closer as possible to those of human cortical bone.^{9,10)} Concerning elastic properties of Ti-Zr alloys, Ho *et al.*¹¹⁾ investigated mechanical properties of a few cast Ti-Zr alloys with Zr concentration of up to 40 mass% (25.9 at%) and reported that their moduli of elasticity in bending were higher than that of pure Ti. Correa *et al.*¹²⁾ measured dynamic elasticity modulus of three Ti-Zr binary alloys containing 5, 10 and 15 mass% Zr at room temperature using a torsion pendulum. They observed the lowest dynamic elasticity modulus of about 86 GPa at 5 mass% Zr (2.7 at% Zr) concentration and increases in the dynamic elasticity modulus with further increases in Zr concentration. There are discrepancies between previously published values of elastic moduli of Ti-Zr binary alloys. Furthermore, no research reports were found where elastic moduli of a series of Ti-Zr binary alloys from a whole range of chemical compositions were investigated.

Knowledge of elastic modulus values of Ti-Zr binary alloys covering the entire range of chemical compositions is particularly important in developing novel Ti-Zr-based multicomponent alloys for a variety of industrial applications including load-bearing biomedical appliances. Since load-bearing biomedical appliances can be fabricated through conventional solidification technologies, such as investment cast hip stems,^{10,13)} the investigation of elastic properties of Ti-Zr binary alloys under as-solidified conditions is meaningful.

The aim of the current study was to determine Young's modulus, shear modulus, bulk modulus and Poisson's ratio values of Ti-Zr binary alloys from the entire range of compositions prepared by arc-melting followed by solidification process and to find a specific composition where low values

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of elastic moduli are obtainable. To evaluate various elastic moduli precisely and non-destructively, an ultrasonic sound velocity measurement technique was employed in the current research. Since elastic properties of metals and alloys are related to their crystal structure, X-ray diffraction was performed to analyze crystal structure of all the samples. Variations of the measured Young's modulus values with composition were discussed and well interpreted in terms of density, Debye temperature and concentration of atoms (number of atoms per unit volume) in each alloy.

2. Materials and Methods

2.1 Sample preparation

Chemical compositions of the experimental Ti-Zr binary alloys are given in Table 1. Button ingots of six experimental Ti-Zr binary alloys containing 20, 40, 50, 60, 70 and 80 at% Zr and pure metals (Ti, Zr) were prepared from pure Ti (99.66%) and pure Zr (99.8%) by the arc-melting method. A total of 30 grams of raw materials for each pure metal and alloy sample was placed in a water-cooled copper hearth in the reaction chamber of an arc-melting apparatus. Purified argon gas with the pressure of approximately 0.1 MPa was used as a protective atmosphere. The starting raw materials were melted for 2 min by argon arc plasma flame with the direct current power of 20 V and 300 A. The button ingots were then turned over and re-melted three times under the same condition to improve chemical homogeneity. Checks on weight losses occurring during arc-melting showed a loss of less than 0.02% for all ingots.

Three plate samples sized $10 \times 10 \times 2 \text{ mm}^3$ were cut out from each as-solidified ingot and their both square faces ($10 \times 10 \text{ mm}^2$) were polished to a mirror-like finish following the conventional metallographic techniques. Optical microscopic observations of all the polished plate samples showed neither porosities nor flaws in all samples. These defect-free samples were then submitted to the following various analyses.

2.2 Density evaluation

The density values of all the Ti-Zr alloys and pure metals (Ti, Zr) were determined by precise measurements of mass and volume of the polished plate samples. The mass of each sample was measured using a high-sensitivity electronic balance (AEM-5200, Shimadzu Corporation, Kyoto, Japan) with an accuracy of $1 \mu\text{g}$. The three dimensions of all the samples

were measured using a micrometer with an accuracy of $1 \mu\text{m}$. Each dimension of a plate sample was measured five times and the average value was used for volume calculation. The density values of the samples were calculated by dividing the mass by the volume. Three polished plate samples were used to obtain the average density value and standard deviation.

2.3 X-ray diffraction

The polished plate samples were mounted in a standard X-ray diffractometer (JDX-3500, JEOL Ltd., Tokyo, Japan) equipped with a rotating-anode Cu target. The diffractometer was operated at a tube voltage of 40 kV and a tube current of 300 mA. A divergence slit with a divergence angle of 1° was used to irradiate the sample surface. X-ray diffraction patterns from each sample were recorded from 20° to 90° (2θ) with a fixed time of 0.5 s and at 0.05° increments to analyze crystal structure of the samples. X-ray optics for the present diffraction analysis showed that the smallest area irradiated by an incident X-ray beam was 10 mm in length (constant value determined by a sample length) and 4.6 mm in width (at $2\theta = 90^\circ$). From the X-ray optics, the area of the sample surface irradiated by the incident X-ray beam increased with decreases in 2θ values. Lattice parameters of the phases in each sample were calculated from observed d -spacing data for all Bragg reflections using the least-squares method in the lattice parameter calculation software (CellCalc, Version 2.20).¹⁴

2.4 Ultrasonic sound velocity measurements and estimation of elastic moduli

Young's modulus, shear modulus, bulk modulus and Poisson's ratio values of the samples were evaluated by measuring the velocities of ultrasonic sound waves traveling in the samples. The velocities of the longitudinal and transverse ultrasonic sound waves were measured at room temperature (25°C) using a longitudinal transducer (20 MHz, 3 mm in diameter) and a shear transducer (20 MHz, 6 mm in diameter) connected to an ultrasonic thickness gage (25DL PLUS, PANAMETRICS-NDT, Waltham, MA, USA). Since the plate samples were as thin as 2 mm in thickness, a small delay element made of polystyrene was used between the longitudinal transducer and the sample. A small amount of propylene glycol was applied as a coupling medium between the longitudinal transducer and the delay element and a small amount of glycerin was applied as a coupling medium between the delay element and the sample. Similarly, a non-toxic, water soluble organic substance of very high viscosity was applied as a coupling medium between the shear transducer and the sample.

The Poisson's ratio (ν), Young's modulus (E), shear modulus (G) and bulk modulus (K) of the samples were calculated according to the following expressions:^{15,16}

$$\nu = (V_L^2 - 2V_T^2)/[2(V_L^2 - V_T^2)] \quad (1)$$

$$E = 2\rho V_T^2(1 + \nu) \quad (2)$$

$$G = E/[2(1 + \nu)] \quad (3)$$

$$K = E/[3(1 - 2\nu)] \quad (4)$$

where, V_L is the velocity of the longitudinal waves, V_T is the velocity of the transverse waves, and ρ is the density of a

Table 1 Chemical compositions of the experimental Ti-Zr binary alloys.

| Sample code | Composition in at% (mass% in parentheses) | |
|-------------|---|-----------|
| | Ti | Zr |
| Ti | 100 | 0 |
| Ti-20Zr | 80 (67.7) | 20 (32.3) |
| Ti-40Zr | 60 (44.0) | 40 (56.0) |
| Ti-50Zr | 50 (34.4) | 50 (65.6) |
| Ti-60Zr | 40 (25.9) | 60 (74.1) |
| Ti-70Zr | 30 (18.4) | 70 (81.6) |
| Ti-80Zr | 20 (11.6) | 80 (88.4) |
| Zr | 0 | 100 |

sample. The measurements of the velocities of both longitudinal and transverse waves were repeated five times for each sample and their average values were used to estimate ν , E , G and K values. Strictly, the eqs. (1) through (4) are applicable to polycrystalline materials with random crystal orientations. In the present samples, some anisotropies of crystal orientations were recognized by X-ray diffraction analysis, as will be mentioned in the following subsection 3.2. This was due to considerably large grain sizes (approximately 300 to 800 μm). However, since the longitudinal and shear transducers of 3 mm and 6 mm in diameters, respectively, were used in the present ultrasonic sound velocity measurements, sufficient numbers of crystal grains were included in the measurements. Accordingly, there were no problems in using the above eqs. (1) through (4) to evaluate various elastic moduli of the present samples.

3. Results

3.1 Density

Figure 1 shows the composition dependence of densities of the Ti-Zr alloys. The evaluated density values for pure Ti and pure Zr were $4.463 \pm 0.002 \text{ g cm}^{-3}$ and $6.491 \pm 0.004 \text{ g cm}^{-3}$, respectively. These values were very close to the published values of 4.5 g cm^{-3} for Ti and 6.50 g cm^{-3} for Zr.⁵⁾ As seen in the figure, density values of Ti-Zr alloys increased with increasing Zr concentration. The density vs. composition curve deviated slightly in a positive direction from the straight line connecting both terminal points for the pure metals.

In this figure and the following similar figures, error bars showing standard deviations assessed from three sample measurements were also presented. However, because the assessed standard deviations were so small in most cases, the corresponding error bars were almost embedded in each data point.

3.2 Crystal structure and lattice parameters

Figure 2 shows X-ray diffraction patterns from the mirror-polished plate samples of the as-solidified pure Ti, pure Zr and a series of Ti-Zr alloys. All Bragg reflections from each sample were identified to be derived from the HCP structure,

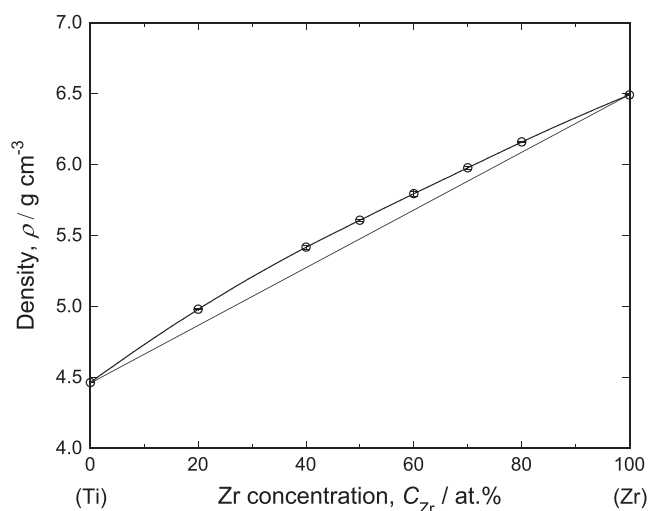


Fig. 1 Composition dependence of densities of the Ti-Zr alloys.

indicating that all samples were in a single-phase structure of the martensitically formed α' -phase under the as-solidified condition. This agrees well with the previous report that the high temperature β -phase with the BCC structure can transform martensitically to the low temperature HCP phase (α') across the entire composition range.⁶⁾ As seen in Fig. 2, some anisotropies of crystal orientations were observed in almost all samples. Optical microscopic observations showed that grain sizes of the present samples were in a range of approximately 300 to 800 μm . As mentioned in the preceding subsection 2.3, the smallest area irradiated by an incident X-ray beam was 10 mm in length (constant value) and 4.6 mm in width at $2\theta = 90^\circ$, and this width obviously increased with decreases in 2θ values. Since this area irradiated by the X-ray beam is not small and comparable to that in the conventional X-ray diffraction analysis, the observed anisotropies of crystal orientations are attributable to the above-mentioned considerably large grain sizes of the present samples.

Since almost all Bragg reflections from each sample were sharp, degree of the possible compositional segregation is considered to be insignificant in all samples. This consideration is supported well by the fact that in the Ti-Zr system differences in liquidus and solidus temperatures are small throughout the entire range of composition.⁶⁾ Therefore, we estimated lattice parameters (a , c) of a unit cell of the α' -phase with the HCP structure by using the observed d -spacing data and the least squares method.¹⁴⁾

Figure 3 shows variations of lattice parameters (a , c) and the volume of a unit cell (V) with Zr concentration. The volume of the unit cell (V) of the α' -phase was calculated according to the following equation:¹⁷⁾

$$V = (\sqrt{3})a^2c/2 \quad (5)$$

The observed a - and c -values for pure Ti were 0.29534 nm and 0.46878 nm, respectively, and those values for pure Zr were 0.32346 nm and 0.51566 nm, respectively. These values were very close to the published values of $a = 0.29508 \text{ nm}$ and $c = 0.46855 \text{ nm}$ for α -Ti¹⁸⁾ and $a = 0.32331 \text{ nm}$ and $c = 0.51491 \text{ nm}$ for α -Zr.¹⁹⁾ The a -value vs. composition curve

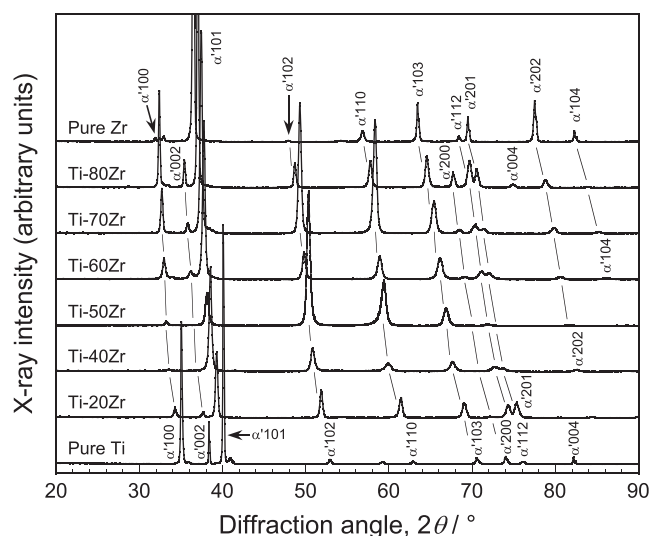


Fig. 2 X-ray diffraction patterns from the Ti-Zr alloys and pure metals (Ti, Zr) prepared by arc-melting followed by solidification process.

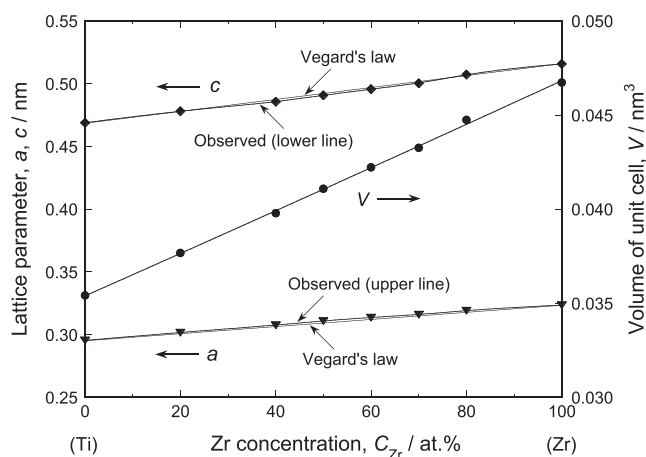


Fig. 3 Variations with Zr concentration of lattice parameters (a , c) and the volume of a unit cell (V) of the α' -phase with the hexagonal close-packed structure.

deviated very slightly in a positive direction from the Vegard's law, whereas the c -value *vs.* composition curve deviated very slightly in a negative direction from the Vegard's law. As a result, the axial ratio (c/a) of the α' -phase gradually decreased with Zr concentration from 1.587 for pure Ti to a minimum value of 1.578 for the Ti-50 at% Zr alloy. Further increases in Zr concentration increased the c/a ratio to 1.594 for pure Zr. The volume of the unit cell of the α' -phase increased almost linearly with Zr concentration (Fig. 3).

The experimental results that the addition of Zr to Ti decreased c/a ratios to a minimum value of 1.578 at the Ti-50 at% Zr composition suggest that the constituent atoms (Ti, Zr) are compressed in the c -direction and must be ellipsoidal in shape. This compression of atoms in the c -direction may possibly be related to the facts that the density *vs.* composition curve deviated slightly in a positive direction from the straight line connecting both terminal points (Fig. 1). Further study will be needed to fully understand this density *vs.* composition behavior and will be published elsewhere in the future.

3.3 Ultrasonic sound velocities and elastic moduli

Velocities of longitudinal and transverse ultrasonic sound waves traveling in the as-solidified samples are presented in Fig. 4 as a function of Zr concentration. In this figure, error bars showing standard deviations from three sample measurements were also presented. However, because the assessed standard deviations were so small, the corresponding error bars were embedded in each data point. The facts that the observed standard deviations were very small demonstrate that the present samples can be considered as isotropic materials in the ultrasonic sound velocity measurements under the current experimental conditions. The alloying addition of Zr to Ti monotonously decreased the velocity of the longitudinal waves from $6003.9 \pm 0.4 \text{ m s}^{-1}$ for pure Ti to $4695.4 \pm 7.3 \text{ m s}^{-1}$ for pure Zr. The observed velocity for pure Zr was in good agreement with the published value of 4698 m s^{-1} for α -Zr.²⁰⁾ A rate of decreases in the velocity of the longitudinal waves with composition was higher in the low Zr concentration ranges compared with that in the high Zr concentration ranges.

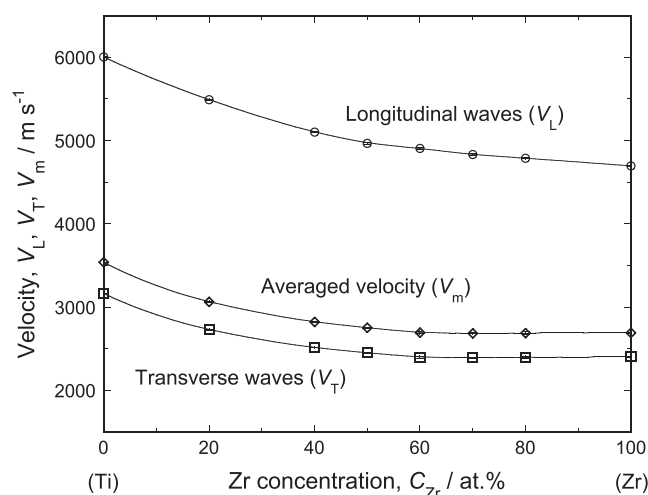


Fig. 4 Variations with Zr concentration of observed velocities of longitudinal and transverse ultrasonic sound waves and the averaged velocity (V_m) calculated according to the eq. (9).

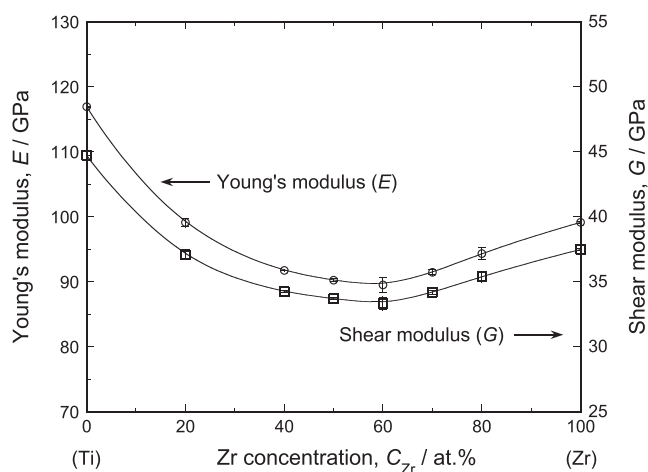


Fig. 5 Variations of Young's modulus (E) and shear modulus (G) with Zr concentration.

Similarly, the alloying addition of Zr to Ti decreased the velocity of the transverse waves from $3165.0 \pm 0.7 \text{ m s}^{-1}$ for pure Ti down to $2391.4 \pm 5.2 \text{ m s}^{-1}$ for the Ti-70 at% Zr alloy. Further increases in Zr concentration increased the velocity of the transverse waves very slightly up to $2402.9 \pm 3.2 \text{ m s}^{-1}$ for pure Zr. This observed velocity for pure Zr was slightly larger than the reported value of 2361 m s^{-1} for α -Zr.²⁰⁾

Figure 5 shows composition dependence of Young's modulus (E) and shear modulus (G) for all the samples estimated using the eqs. (2) and (3), respectively. Young's modulus for pure Ti was $116.9 \pm 0.1 \text{ GPa}$, which was in good agreement with the published values of 117 GPa ²¹⁾ and 114.2 GPa .²²⁾ Young's modulus for pure Zr was $99.1 \pm 0.2 \text{ GPa}$, which agreed well with the previously reported value of 97.6 GPa ²²⁾ and 96.6 GPa .²⁰⁾ The alloying addition of Zr to Ti was found to decrease effectively Young's modulus with the minimum value of $89.5 \pm 1.0 \text{ GPa}$ being recorded at the composition Ti-60 at% Zr (Fig. 5).

Shear modulus for pure Ti and pure Zr were observed to be 44.7 GPa and $37.5 \pm 0.1 \text{ GPa}$, respectively. The observed

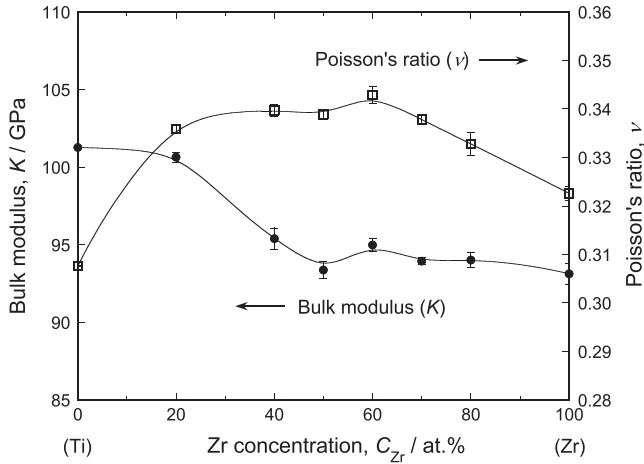


Fig. 6 Variations of bulk modulus (K) and Poisson's ratio (ν) with Zr concentration.

shear modulus for pure Ti was very close to the published values of 44.8 GPa²¹⁾ and 45 GPa.²³⁾ Similarly, the observed value for pure Zr was in good agreement with the previously reported values of 36.1 GPa^{22,24)} and 36.3 GPa.²⁰⁾ The composition dependence of the shear modulus was very similar to that of Young's modulus and the minimum shear modulus of 33.3 ± 0.4 GPa was recorded at the same composition Ti-60 at% Zr (Fig. 5).

Figure 6 shows variations of bulk modulus (K) and Poisson's ratio (ν) with Zr concentration estimated using the eqs. (4) and (1), respectively. The bulk modulus values for pure Ti and pure Zr were 101.3 ± 0.01 GPa and 93.1 ± 0.7 GPa, respectively. These observed values coincided well with the previously reported values of 102 GPa for α -Ti^{25,26)} and 92 GPa for α -Zr.²⁷⁾ The observed bulk modulus values for Ti-Zr binary alloys showed fairly mild but characteristic variations with composition. That is, a slight decrease in bulk modulus occurred when the concentration of Zr was increased from 20 to nearly 50 at% and further increases in Zr concentration did not change the bulk modulus greatly. The bulk modulus for the Ti-50 at% Zr alloy was observed to be 93.4 ± 0.5 GPa, which was slightly lower than the theoretically predicted value of 97.8 GPa for an α -phase Ti-Zr alloy with this composition.²⁸⁾

With increasing Zr concentration Poisson's ratio of a sample increased from 0.308 for pure Ti to a maximum value of 0.343 ± 0.002 for the Ti-60 at% Zr alloy. Further increases in Zr concentration decreased Poisson's ratio down to 0.323 \pm 0.001 for pure Zr (Fig. 6).

4. Discussion

The good agreement of the observed various elastic moduli for pure metals (Ti, Zr) with the previously published data certifies the validity of the elastic property data for the present Ti-Zr binary alloys. We will interpret the observed variations of Young's modulus with composition in terms of density, Debye temperature and concentration of atoms in a solid which are all considered to affect elastic properties of an alloy. The Debye temperature is an important parameter of a solid and is found in equations describing properties which arise from

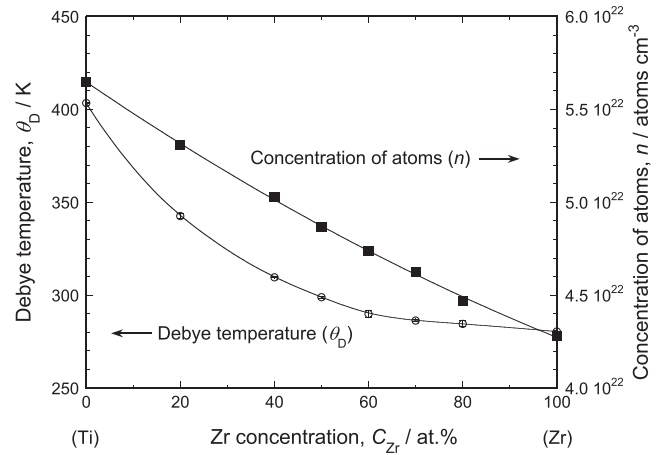


Fig. 7 Variations of estimated concentration of atoms (n) and Debye temperature (θ_D) with Zr concentration.

atomic vibrations, and in theories involving phonons.²⁹⁾ In fact, the velocity of ultrasonic sound waves traveling in a substance is known to be related to the Debye temperature. Young's modulus, E , of a substance is related to the Debye temperature, θ_D , as follows:³⁰⁾

$$E \sim \rho \theta_D^2 n^{-2/3} \quad (6)$$

where, ρ is the density of the substance and n is the concentration of atoms, i.e., number of atoms per unit volume of the substance. The relation (6) indicates that the smaller the ρ , the lower the θ_D , and the larger the n , the lower the Young's modulus of the substance. Since the density values of the Ti-Zr alloys and the component pure metals have been measured in the present study and presented in Fig. 1, we estimated concentration of atoms (n) and Debye temperature (θ_D) of each alloy.

The n value for hexagonal crystal lattice can be calculated using number of atoms in a unit cell and volume of the unit cell according to the following equation:¹⁷⁾

$$n = 2 / \{ (\sqrt{3}) a^2 c / 2 \} \quad (7)$$

where, a and c are lengths of a - and c -axes of the unit cell, respectively. The results of this calculation are given in Fig. 7 as a function of Zr concentration. The concentration of atoms monotonously decreased from 5.648×10^{22} atoms cm^{-3} for pure Ti to 4.280×10^{22} atoms cm^{-3} for pure Zr. This monotonous decrease in concentration of atoms with Zr concentration is well interpreted in terms of the fact that the volume of the unit cell of the α' -phase increased almost linearly with Zr concentration (Fig. 3).

One of the standard methods of calculating the Debye temperature, θ_D , is from elastic constant data, since θ_D is proportional to the sound velocity (averaged), V_m , by the equation

$$\theta_D = (h/k) [(3qN\rho)/(4\pi M)]^{1/3} V_m \quad (8)$$

where, h is Planck's constant, k is Boltzmann's constant, N is Avogadro's number, ρ is the density, M is the molecular weight of the solid and q is the number of atoms in the molecule.^{20,29)} The averaged sound velocity, V_m , in the eq. (8) can be calculated according to the following equation:²⁹⁾

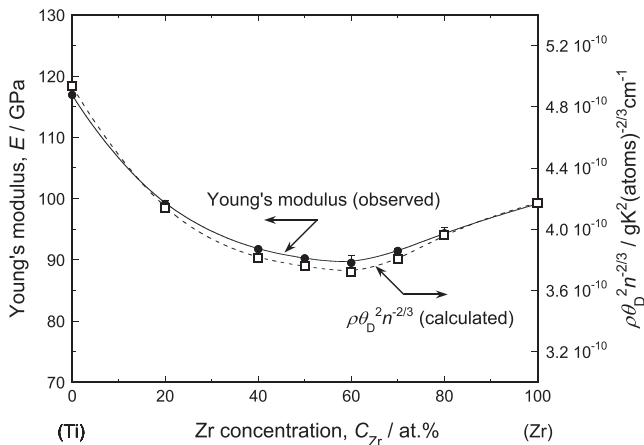


Fig. 8 Comparison of composition dependences of the observed Young's modulus (solid line) and the calculated $\rho\theta_D^2 n^{-2/3}$ values (dashed line).

$$V_m = [(2/3V_T^3) + (1/3V_L^3)]^{-1/3} \quad (9)$$

where, V_T and V_L are the velocities of the transverse and the longitudinal ultrasonic sound waves, respectively.

We calculated each sample's V_m value according to the eq. (9) and presented the results of this calculation in Fig. 4 as a function of Zr concentration. The V_m value decreased with increasing Zr concentration from 3538.7 m s^{-1} for pure Ti to 2684.3 m s^{-1} for the Ti-70 at% Zr composition. However, further increases in Zr concentration increased V_m values very slightly up to 2691.8 m s^{-1} for pure Zr.

Using these calculated V_m values, we estimated the Debye temperature, θ_D , of each sample according to the eq. (8). For pure metals (Ti, Zr), the atomic weight of each element was used as M value in the equation ($M = 47.867$ for Ti and 91.224 for Zr).³¹⁾ For each alloy, a compositionally averaged atomic weight was used as M value. The results of this estimation for θ_D are plotted in Fig. 7 as a function of Zr concentration. The Debye temperature for pure Ti was estimated to be 403 K which was comparable to the published value of 385 K for α -Ti.³²⁾ Similarly, the Debye temperature for pure Zr was estimated to be 280 K which was in good agreement with the reported value of 275.9 K for α -Zr.²⁰⁾ These good agreements of our estimated Debye temperatures for pure metals (Ti, Zr) with the previously published values support the validity of the current estimation of the Debye temperatures for the experimental Ti-Zr alloys. It was found that the alloying addition of Zr to Ti significantly lowered the θ_D value and that this effect of lowering the θ_D was substantially greater in the low Zr concentration ranges (Fig. 7).

Using the estimated concentration of atoms (n), Debye temperature (θ_D), and observed density (ρ), we calculated $\rho\theta_D^2 n^{-2/3}$ value in the relation (6) for each alloy and pure metal and plotted the results of this calculation in Fig. 8 as a function of Zr concentration. For comparison, the observed Young's modulus values were also presented. As one can see, the fitting of both curves is satisfactorily good and the composition where the lowest Young's modulus is observed coincides very well. This certifies that the quantity $\rho\theta_D^2 n^{-2/3}$ is a good measure in predicting the trends of variations with composition of Young's modulus of the Ti-Zr alloys throughout the entire range of composition. In summary this study sug-

gests that a particular composition at which the lowest Young's modulus is obtainable can be predicted when density, Debye temperature, crystal structure, and lattice parameters of a series of alloys are known.

The current study found the lowest Young's modulus of 89.5 GPa at the composition Ti-60 at% Zr. This value is significantly lower than those for the practically used pure Ti and Ti-6Al-4V alloy. However, it is still high in comparison with the value for human cortical bone (15.2 to 40.8 GPa depending on strain rate³³⁾). The further study will be required to develop novel titanium alloys with reduced Young's moduli. In such cases, the current study is expected to be helpful in designing compositions of new Ti-Zr-based alloys with lower Young's moduli for biomedical applications.

5. Conclusions

Elastic moduli of as-solidified Ti-Zr binary alloys from the entire range of composition were investigated by means of ultrasonic sound velocity measurements and the following conclusions were drawn.

The alloying addition of Zr to Ti effectively lowered both Young's modulus (E) and shear modulus (G) with their minimum values of $89.5 \pm 1.0 \text{ GPa}$ and $33.3 \pm 0.4 \text{ GPa}$, respectively, being recorded at the same composition Ti-60 at% Zr. On the other hand, bulk modulus (K) decreased slightly when the concentration of Zr was increased from 20 to nearly 50 at% and further increases in Zr concentration did not change the bulk modulus greatly. The observed variations of Young's modulus with Zr concentration in the entire range of composition were well interpreted in terms of density (ρ), Debye temperature (θ_D), and concentration of atoms (n), i.e., number of atoms per unit volume of each alloy. The quantity $\rho\theta_D^2 n^{-2/3}$ was revealed to be a good measure in predicting the tendency of variations of Young's modulus with composition in this binary system.

Acknowledgments

The authors thank Mr. Shun Ito, Ms. Akiko Nomura, and Mr. Kazuo Obara of Institute for Materials Research, Tohoku University, Sendai, Japan for their contribution to sample preparation. Acknowledgment is also given to the Center for Instrumental Analysis of Kyushu Institute of Technology, Kitakyushu, Japan, for X-ray diffraction analysis. One of the authors, T.S., expresses gratitude to the inter-university cooperative research programs (Proposal Numbers 06G0055, 07G0045, 13G0014) of the Cooperative Research and Development Center for Advanced Materials, Institute for Materials Research, Tohoku University, Sendai, Japan. This work was supported in part by The Grant-in-Aid for Scientific Research from The Ministry of Education, Culture, Sports, Science and Technology in Japan under Grants (C) 16591960 and (C) 19592250.

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