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Microstructural Characterization, Mechanical Properties, and Artificial Neural Network-Based Prediction of β Titanium Alloys for Biomedical Applications

Aline Raquel Vieira Nunes[1,*], Ramon de Attayde Barros de Souza[1], Lusiene Thaiane dos Santos Tannis [1], Ana Isabel de Carvalho Santana[1], Caio Marcello Felbinger Azevedo Cossú[1], João de Ataíde Garcia[1], Sinara Borborema[1], Luiz Henrique de Almeida[2]

[1]Rio de Janeiro State University, Rio de Janeiro, RJ, Brazil; [2]Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil;
*aline.nunes@uerj.br

Introduction

Metastable β titanium alloys with low Young's modulus are candidates to replace Ti-6Al-4V in orthopedic implants. The stability of the β phase can be estimated by the molybdenum equivalent ([Mo]eq), in which Zr is treated as neutral [1] or as a β stabilizer [2]. The effect of Zr on Ti-Nb-Mo alloys after cold deformation is not fully understood. This work evaluated the effect of Zr on the microstructure and mechanical properties of Ti-24Nb-4Mo-xZr (wt.%) alloys. The alloys were arc melted, homogenized at 1000 °C for 24 h, water quenched and cold rolled to 90 % thickness reduction. The microstructure was characterized by optical microscopy (OM), scanning electron microscopy (SEM) and X-ray diffraction (XRD). The Young's modulus was measured by impulse excitation and the hardness by Vickers microhardness. XRD indicated a β matrix with reflections consistent with α″ martensite in the three alloys. The alloys showed elongated grains crossed by deformation bands. As the Zr content increased, the Young's modulus and microhardness decreased, thus, the HV/E ratio increased from 4.60 to 4.77 HV/GPa, above the value estimated for Ti-6Al-4V (3.08 HV/GPa). An artificial neural network (ANN) was trained on 336 titanium alloys described by 29 compositional and processing variables. The selected neural network (29-64-32-1, dropout = 0.2) achieved R^2 = 0.45 and a mean absolute error (MAE) of 10.8 GPa in 5-fold cross-validation.

Objectives

To evaluate the effect of Zr (0, 3 and 6 wt.%) on the microstructure, Young's modulus, microhardness and HV/E ratio of Ti-24Nb-4Mo alloys cold rolled to 90 %, and to compare the measured modulus with the values predicted by an artificial neural network.

Methodology

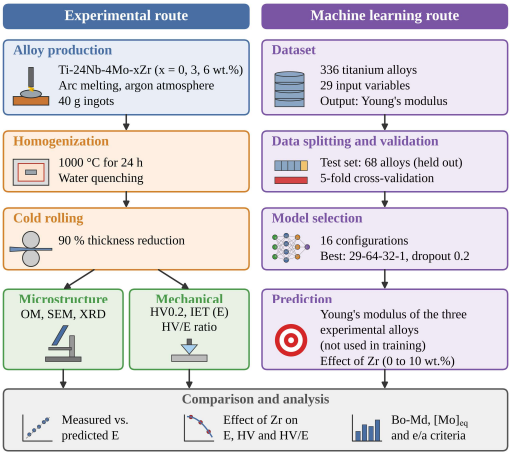

Figure 1. Study workflow. Experimental route: production, homogenization and cold rolling of the alloys, followed by microstructural and mechanical characterization. Machine learning route: dataset, data splitting, model selection and prediction of the Young's modulus of the three alloys.

Results and Discussion

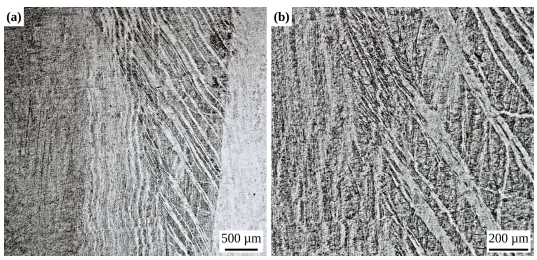

Figure 2. Optical micrographs of Ti-24Nb-4Mo-6Zr after 90 % cold rolling: (a) elongated grains crossed by deformation bands; (b) intersecting bands forming a fibrous structure inside the deformed grains. Kroll's reagent.

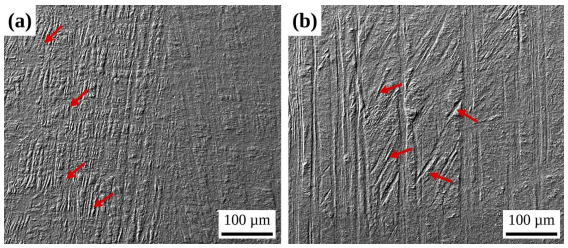

Figure 3. SEM images (secondary electrons) of Ti-24Nb-4Mo-6Zr after 90 % cold rolling: (a, b) 500×. Arrows: acicular and lenticular features consistent with α″ martensite or deformation twins, which SEM alone does not distinguish.

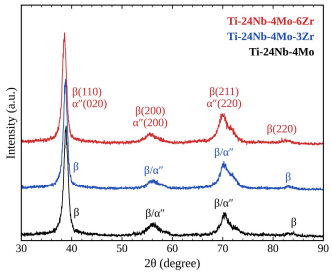

Figure 4. XRD patterns after 90 % cold rolling. β (110) is the main peak. Shoulders near 2θ = 38°, 58° and 72° were assigned to α″ martensite.

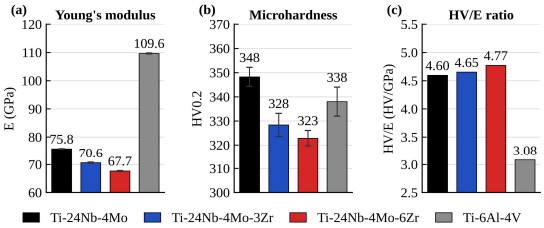

Figure 5. (a) Young's modulus (impulse excitation), (b) Vickers microhardness and (c) HV/E ratio, compared with Ti-6Al-4V. Zr lowers E, and HV/E increases from 4.60 to 4.77 HV/GPa. E error bars: SD of 12 measurements on one specimen. Axes do not start at zero.

Table 1. Measured and ANN-predicted Young's modulus, hardness and HV/E.

Alloy	E measured (GPa)	E ANN (GPa)	Error GPa (%)	HV0.2	HV/E (HV/GPa)
Ti-24Nb-4Mo	75.76 ± 0.08	58.28	17.48 (23.1)	348.24 ± 3.94	4.60
Ti-24Nb-4Mo-3Zr	70.59 ± 0.20	57.43	13.16 (18.6)	328.38 ± 4.78	4.65
Ti-24Nb-4Mo-6Zr	67.65 ± 0.15	56.63	11.02 (16.3)	322.86 ± 3.23	4.77
Ti-6Al-4V [3]	109.62 ± 0.16	n.a.	n.a.	338 ± 6	3.08

E: mean ± SD of 12 measurements on one specimen. HV: mean ± SD of the indentations; Ti-6Al-4V hardness from [3]. Error: E measured − E predicted (relative error in parentheses).

Conclusions

- After 90 % cold rolling, all alloys showed a deformed β matrix with XRD reflections consistent with α″ martensite.
- Zr increased the apparent β lattice parameter (3.273 to 3.296 Å) and decreased the Young's modulus (75.8 to 67.7 GPa), 38 % below that of Ti-6Al-4V.
- The Zr-free alloy was the hardest (348 HV0.2). The 3Zr and 6Zr alloys had close values (328 and 323 HV0.2).
- Among the tested specimens, Ti-24Nb-4Mo-6Zr had the lowest modulus and the highest HV/E ratio (4.77 HV/GPa).
- The predictions indicated a decrease in Young's modulus from 58.28 GPa to 57.43 GPa and 56.63 GPa as the zirconium fraction increased from 0% to 3% and 6%, respectively, suggesting that the neural network was able to capture this trend.

References and Acknowledgments

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[3] NUNES, A. R. V. *et al.* **In Vitro Models**, 2026. DOI: 10.1007/s44164-026-00130-0.

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