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Artificial neural network based optimization of prerequisite properties for the design of biocompatible titanium alloys

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ABSTRACT

The objective of the current study was to design titanium alloys by optimizing tensile strength, yield strength, modulus of elasticity and biocompatibility using the artificial neural network (ANN) and recursive partitioning (RP) models. The database of 308 titanium alloys served as the basis of the model with alloy composition and processing parameters as inputs and each property to be optimized as the target. Levenberg-Marquardt back propagation was used to train the ANN model. RP model was used to elucidate different thresholds of alloying elements that are decisive of biocompatibility. The sensitivity analysis of ANN model revealed that Ta and Nb when used at very high concentrations (30–35%), their tensile and yield strength are higher. With the increase in the concentration of Ta and Nb, the modulus of elasticity was shown to decrease and at high concentrations, modulus of elasticity reaches to that of cortical bone. The RP model showed that these two alloys are safe. Hence, we have generated ANN simulations of Ti-xNb-yTa ternary system to ascertain the optimal combination of Ta and Nb that can provide higher tensile and yield strengths and lower modulus of elasticity. These simulations were compared with already developed alloys with these combinations. To conclude, ANN-based optimization of prerequisite properties facilitated timely and cost-effective solutions in the design of biocompatible titanium alloys.

1. Introduction

Pure titanium and certain titanium alloys are being used as biomaterials for orthodontic and orthopedic implants [1]. Lower density, higher strength, lower modulus of elasticity and lesser cytotoxicity are the parameters that dictate the success of an implant. Alpha titanium alloys have low to medium strength and good ductility. The strengths of alpha + beta titanium alloys are medium to high with loss of ductility in the weld area. Beta titanium alloys have higher strength and have a lower modulus of elasticity and shear modulus compared to alpha and alpha + beta titanium alloys [2,3].

Initially, Ti-6Al-4V was used as a biomaterial because of its high strength. However, this alloy exhibits following limitations as biomaterial: (i) it has a higher modulus of elasticity than the human bone (105–110 GPa vs. 20 GPa) [4]; (ii) it has high dissolvability inside the human body; (iii) exhibits toxicity due to V and its oxides [5,6]; (iv) induces pro-inflammatory and osteolytic response [7].

Ti-6Al-7Nb and Ti-5Al-2.5 Fe alloys with mechanical properties similar to Ti-6Al-4V ELI were developed in order to overcome these limitations. However, Al also was reported to induce necrosis [3]. Hence, efforts are made to substitute Al with Zr and V with Nb or Ta in order to retain similar strength and simultaneously attain low modulus of elasticity [8]. Alpha stabilizers such as Al, Sn, Si, and O stabilize close-packed hexagonal alpha phase. Beta stabilizers such as Mo, V, Cr, Zr, and Fe stabilize body-centered cubic beta phase. The safety and biocompatibility of beta stabilizers such as Nb, Ta, Ti, and Zr resulted in the development of beta titanium alloys as the preferred implant materials that can withstand stress-shield effect and have high fatigue resistance and resistance to wear and tear [3].

Thermomechanical processing parameters such as solution treatment and ageing process comprising β solid solutioning, cold deformation, continuous rapid heating and ageing can be optimized to obtain a fine-grain microstructure with a controlled β grain size that ensures higher strength with reasonable ductility [9].

In order to predict the mechanical properties of titanium alloys based on the alloy composition, heat treatment parameters, and work temperature, Malinov et al. developed an artificial neural network (ANN) model [10]. Genetic algorithms and fuzzy network models were employed for the design of alloys having a low modulus of elasticity, high strength and biocompatibility by optimizing the alloy composition and processing parameters [11–13]. In the current study, we have integrated the existing experimental data on the titanium alloys to

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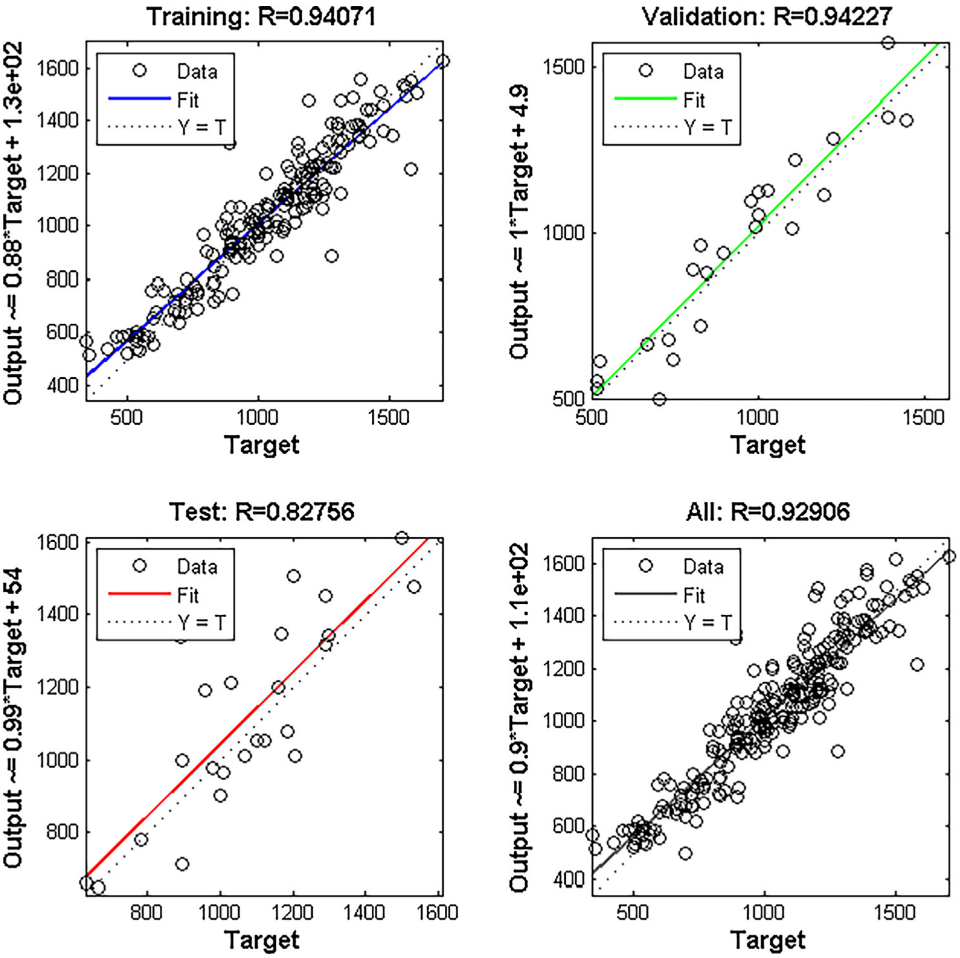

Fig. 1. Correlation between the experimental and the predicted tensile strength. This illustrates correlation between the experimental and the predicted tensile strength in the training, validation, testing and whole data sets.

develop ANN models that can predict tensile strength, yield strength, and modulus of elasticity based on the alloy composition, thermomechanical processing and microstructure. Such models provide a platform for further experimentation and design of new biomaterials. A recent study by Liu et al. reported that Nb-25Ti-xTa (x = 10, 15, 20, 25, 35 wt%) alloys have good biocompatibility, increase in Ta increases the tensile strength and modulus of elasticity can be reduced by increasing sintering temperatures to facilitate homogeneous beta phase [14]. Another recent study on Ti-Nb17-Ta6 biocompatible alloy showed that addition of small quantities of Fe and O stabilize the beta phase in the treated solution condition thus increasing the strength and decreasing the modulus of elasticity [15]. These recent studies prompted us to use Ti-xNb-yTa as the model system for the development of biocompatible titanium alloys by optimizing x and y (wt%).

2. Materials and methods

2.1. Collection of experimental data

The experimental data of 308 titanium alloys on the alloy composition, thermomechanical processing, microstructure and mechanical properties were collected using www.matweb.com, material property handbook of titanium alloys [16] and other published literature [17,18]. The alloy composition (wt% of Mo, V, Al, Zr, Nb, Ta, Mn, Cr, Fe, Sn, Si, O, N, C, H, Ni, Y, Pd and Ru), and thermomechanical processing (heat treatment digitized, solution treatment, ageing, annealing and forging) were used as input variables. The digitization of heat treatment was done as follows: no heat treatment, annealing (β), annealing (α + β), annealing (α), solution treatment (β), solution treatment (α + β), solution treatment (β) + ageing, solution treatment (α + β) + ageing, duplex annealing were digitized as 0, 1, 2, 3, 4, 5, 6, 7 and 8. The mechanical properties namely tensile strength (MPa), yield strength (MPa) and modulus of elasticity (GPa) were used as target variables.

2.2. Development of artificial neural network models

The experimental data were randomly segregated into training data, testing data and validation data. The training data comprised 70% alloys and testing and validation data had 15% alloys in each group. A two-layer feed-forward network with sigmoid hidden neurons and linear output neurons was developed. The neural network was trained using Levenberg-Marquardt back propagation. The number of hidden neurons was optimized by trial and error until least root-mean-square error was obtained. After training the neural network, the regression plots representing regression coefficient (r) corresponding to training, validation, testing and whole dataset were obtained. Once the model was trained, the generated code will be used to predict unknown targets based on given inputs. The ANN models were developed using MATLAB R 2013a.

2.3. Biocompatibility assessment

Based on the published data for alloying elements [19], the coefficient of fibroblast outgrowth and the relative growth rate of L929 cells were assessed as described earlier [20]. Based on these criteria, the

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