INVESTIGATION OF MECHANICAL PROPERTIES OF HAP COATINGS COATED ON TI6AL4V MATERIAL BY ANSYS PROGRAM

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ABSTRACT

Biomaterials are synthetic or natural materials used to support the functions of living tissues in the human body structure and are continuously or periodically in contact with body fluids (eg blood). Biomaterials are used for repair of damaged tissue and organs by implantation, must be compatible with the body in order to perform the required functions. In this study, titanium alloy, which has the best biocompatibility, was used as a base material for long-term implantation (placing it in the skin). In addition, hydroxyapatite coating was performed on the surface of Ti6Al4V material using aminoacetic acid - sodium aminoacetate buffer system. Coatings were modeled with the ANSYS program to examine the mechanical properties of the resulting coatings. Mechanical properties such as tensile analysis, natural frequency, etc. of the coating have been investigated in order to determine the resistance against the mechanical effects that the coating applied by the modeling can be exposed to in use.

Keywords: Coating, Hydroxyapatite (HAp), FEM

HAP KAPLANAN TI6AL4V MALZEMELERİN ANSYS PROGRAMI İLE MEKANİK ÖZELLİKLERİNİN İNCELENMESİ

ÖZET

Biyomalzemeler, insan vücut yapısındaki canlı dokuların fonksiyonlarını yerine getirmek veya desteklemek maksadıyla kullanılan sentetik ya da doğal malzemeler olup sürekli olarak ya da belirli aralıklarla vücut akışkanları ile (örneğin kan) temas ederler. İmplantasyon işlemiyle hasar gören doku ve organların tamiri için kullanılan biyomalzemelerin gerekli istenen işlevleri yerine getirebilmesi için vücut ile uyumlu olması gerekmektedir. Çalışmada altlık malzemesi olarak, uzun süreli implantasyonda (deri içine yerleştirmede) en iyi biyouyumluluğa sahip olan titanyumun alaşımı kullanılmıştır. Bu çalışmada aminoasetik asit – sodyum aminoasetat tampon sistemi kullanılarak Ti6Al4V malzeme yüzeyine hidroksiapatit kaplamanın malzemeler sonlu elemanlar metoduyla modellenmiştir. Yapılan modelleme ile uygulanan kaplamanın kullanım yerlerinde maruz kalabileceği mekanik etkilere karşı dayanımını belirleyebilmek için kaplamanın gerilme analizi, doğal frekansı gibi mekanik özellikleri incelenmiştir.

Anahtar kelimeler: Kaplama, Hidroksiapatit (HAp), SEM

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1. INTRODUCTION

Degenerative and inflammatory diseases of fractures, bones and joints, congenital and acquired deformities, spinal deformities, primary or metastatic tumoral diseases of the skeletal muscle system affect millions of people every year. These diseases often cause tissue and organs to be damaged and even to lose their function. These bruises and loss of function often indicate the need for surgical intervention. Metal - based biomaterials are the most suitable materials for the mechanical loadings of the skeletal - muscle system and the mechanical properties of this system [1].

Ceramic materials used in orthopedic and dental applications show biocompatibility. These materials, which are expressed as ceramics, have advantages which are similar to the tissues. The best material providing these properties is hydroxyapatite [2]. Hydroxyapatite (HA) is a biomaterial that contains calcium and phosphate groups in the apatite group of bioactive ceramics. By virtue of this feature, it is chemically resistant to the apatite structure of the bone and to other hard tissues. However, since hydroxyapatite cannot meet the values of bone alone in terms of its mechanical properties, it is generally used on the base material [3, 4].

Application of HA coating on metal surface; to combine the high biocompatibility and bioactivity of HA with the mechanical properties of metallic materials to achieve bone / implant fixation via chemical binding [5, 6].

There are various methods for preparing these coatings. Sol-gel and biomimetic techniques have been applied, including coating with dipping, spray coating, pulsed laser precipitation, electrophoretic coating, plasma spray and thermal spray coating such as HVOF (High Velocity Oxy-Fuel) [7, 8].

In this work, Ti6Al4V alloy which is the most preferred as base material is used. Biomimetic method was preferred for coating and a synthetic body fluid (SBF) was used in the same values as the ion values in human blood plasma. In this study, plating of substrate materials was carried out on Ti6Al4V alloy for 24, 48, 72 and 96 hours using Aminoacetic Acid-Sodium Aminoacetate buffer system environment with biomimetic technique for the first time.

In addition to working, the coatings are modeled with the finite element method in ANSYS program. The mechanical properties of the modeled coatings are investigated using this program.

2. MATERIAL AND METHOD

2.1 Selection of implant material

In the experiment, Ti6Al4V substrate material, which is frequently used as implant material in the plating process, is used in dimensions of 10x10x1.2 mm. Table 1 shows the chemical composition of the substrate material and Table 2 gives the mechanical properties.

Element	%
Ti	The Rest
С	0,005
N	0,003
Fe	0,1
0	0,09
V	3,87
Al	6,21
Н	<,0005
Y	<,001
Other	<,3

Table 1. Ti6Al4V weight chemical composition of alloy (ASTM F 1044-99) [3]

Table 2. Mechanical properties of Ti6Al4V material [5]

Material	Yield Stress	Tensile Stress	Strain %	Reduction Ratio
	(MPa)	(MPa)		%
Ti6Al4V	883	960	13	50

2.2 Preparation of coating

In the preparation of coating part, firstly the base material was sanded. The sanded materials were washed sequentially with pure water, then placed in acetone, washed again with distilled water, and placed in an ultrasonic bath. In the ultrasonic bath, the cleaned based materials were kept at 40 °C for 24 hours to provide surface activity in 100 mL 5M NaOH + 0.5 mL 35% H2O2 solution and sodium titanate hydrolyzate formation. After the surfaceactivated substrates were washed with pure water, the material was allowed to dry at 60 °C. Aluminum foil wrapped material that cannot get air is kept at 600 °C temperature for 1 hour and cooled to room temperature again. The salts of the amounts in Table 3 for SBF were dissolved in 2 L of the solution by mixing in the magnetic stir bar in a 2 L beaker in 1.5 L of purified water. The solution was heated to 37 °C and added to 1 M glycine solution and measured by pH meter to pH 8. The pH of the solution was lowered to 7.4 by addition of MgCl2.6H2O and CaCl2.2H2O salts and the glycine solution was added again and the volume was reduced to 2 L by the addition of pure water. The coating process was carried out by biomimetic methods on substrates prepared at 37 °C for 24, 48, 72, 96 hours and kept in SBF. At the end of the process, the materials removed from the solutions were rinsed with pure water and left to dry at 60 °C [7]. Table 3 shows the amount of salt used when preparing the SBF.

Table 3. Inorganic salts and amounts in SBF (total volume = 2L) [7]

Material	mg/Mmol	Amount (mg/2L)	Mmol/L
KCl	74,55	746,0	K ⁺ : 5; Cl ⁻ : 5
NaCl	58,44	10519,2	Na ⁺ :90; Cl ⁻ :90
Na ₂ HPO ₄ H ₂ O	177,99	356,0	HPO ₄ ²⁻ :1; Na ⁺ : 2
Na ₂ SO ₄	143,04	142,0	SO ₄ ²⁻ :0,5; Na ⁺ : 1

N UCO	94.01	15266	1100 - 27 M + 27

Nanco ₃	04,01	4550,0	$\Pi CO_3 . 2/, Na . 2/$
Na-glycinate (Na-	97,05	4313,4	Na ⁺ :22
aminoacetate)			
$CaCl_2.2H_2O$	147,02	735,2	$Ca^{2+}: 2,5; Cl^{-}: 5$
MgCl ₂ .6 H ₂ O	203,31	610,0	Mg ²⁺ : 1,5; Cl ⁻ : 3
Glycine (>99%) 1M	75,06		
(Aminoacetic acid)			

These implants, given the manufacturing method and whose coating thicknesses vary according to the waiting time, are modeled by the finite element method as the coating material and the buffer material have the same production thickness. Table 4 gives the coating thicknesses and Table 5 gives the modulus of elasticity that materials used are taken.

Table 4. Average coating thicknesses [7]

HA Waiting Time	Coating Thicknesses
(Hour)	(µm)
24	4,13 ±0,255
48	4,73 ±0,157
72	$5,47 \pm 0,098$
96	5,55 ±0,102

Table 5. Elasticity Modules of Coatings for Waiting Times [9]

HA Waiting Time	Modulus of Elasticity
(Hour)	[E] (GPa)
24	1,238
48	0,351
72	0339
96	0,173

The implant material was modeled as a composite material with the aid of the ANSYS program and fixed at four sides (Figure 1), taking into account the substrate material measured previously and the coating thicknesses and modulus of elasticity formed at the end of the 24, 48, 72 and 96 hour waiting periods. The penetration depths, maximum stress values and stress distributions of these samples were plotted under equal conditions with the application of 1 N force from the midpoint of each sample.



Figure 1. Finite Element Model

3. RESULTS

The penetration depth and stress distribution plots of each sample of 4 different waiting times of 10x10x1.2 mm size under 1 N load are similar. Figure 2 shows the deformation distributions of samples under 1 N load and Figure 3 shows the general behavior of stress distributions.



Figure 2. Deformation Distribution



Although the tensile distribution graphs were obtained in a similar manner, differences in penetration depth and maximum stress values of the 4 different samples obtained by 24, 48, 72 and 96 hour stand-offs resulted from the thickness and elasticity modulus of the coatings. Figure 4 shows the variation of penetration depths corresponding to the waiting times. Figure 5 shows the Von Mises stress values corresponding to different waiting times and these waiting times. According to this graph, by increasing the coating time from 24 hours to 96 hours, the tensile value carried by the material reaches only 16% of the initial value.



Figure 4. Penetration Depths



Figure 5. Von Mises Stresses

In addition to these results, how the first natural frequency of the sample implant changes with respect to the waiting times is also examined. The first natural frequencies corresponding to the different waiting times of the samples are given in Figure 6. According to this graph, it is observed that the first natural frequency value is in the decreasing behavior by increasing the waiting time.



Figure 6. First Natural Frequencies

4. CONCLUSIONS

As a result of this study, hydroxyapatite coated surface of Ti6Al4V material which is compatible with blood plasma using amino acetic acid - sodium aminoacetate buffer system was modeled in ANSYS program. Mechanical properties such as tensile, natural frequency, etc. have been investigated to determine the resistance to applied mechanical effects of coatings. It

is known that as the waiting time from previous researches increases, the coating thickness increases and the elastic modulus of the coating decreases. In the analysis of these data, penetration depth increased and Von Mises tensile value decreased as the waiting time increased. In addition, the natural frequency values of the implants decreased as the waiting time increased.

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