The Influence of Surface Roughness on Biocompatibility and Fatigue Life of Titanium Based Alloys

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Abstract. This article deals with the effect of treatment on the mechanical properties of biocompatible alloys. In the case of implants, it is desirable to ensure good biocompatibility. Generally, the environment in the body is very aggressive and implants can quickly degrade due the corrosion. The process of corrosion leads to the release of harmful particles into the body. Other reasons for rejection of the implants, is their coverage bacterial plaque. Another reason for the rejection of the implant may be a smooth surface. In some cases, the tissue does not adhere to the smooth surface of the implant, in this regions occurs an accumulation of body fluids. This problem can be solved with a rough surface. From the viewpoint of fatigue resistance, the rough surface containing grooves and holes has a negative influence on the fatigue resistance against mechanical loading. The rough surface can be produced by machining or asymmetric deposition of particles of oxides, nitrides or other particles on surface. In this work the formation and propagation of fatigue cracks in the material with granular surface is analysed. The formation and growth of fatigue crack originated from granular surface is simulated. Also, experimental studies were carried out.

1. Introduction
In the case of implants used in medicine, it is desirable to ensure good biocompatibility\textsuperscript{[1,2,3]}. The biocompatibility is important property of materials used for construction of medical implants. Generally, the environment in the human body is very aggressive and implants can quickly degrade due the corrosion. The process of corrosion leads to the release of harmful particles into the body. For this reason, for example, titanium alloys with niobium content are preferred before alloys containing harmful vanadium or nickel. The corrosion can be reduced through appropriate surface finishes. Another important problem is the ability of the human body to accept implant. The body is trying to push out foreign objects. One of the reasons for rejection of the implants is their coverage bacterial plaque. Another reason for the rejection of the implant may be a smooth surface. In some rare cases (1% of cases in maximum), the tissue does not adhere to the smooth surface of the implant, in this regions occurs an accumulation of body fluids. In the area of fluid accumulation often occurs secondary inflammation. Experiments realized on animals shows that the body accepts better implants with a rough surface. This phenomenon can be explained by better adherence of tissue to the rough surface of implant. The rough surface can be produced by machining. From the viewpoint of fatigue resistance, grooves on the machined rough surface have a negative influence on the fatigue resistance against mechanical loading. The rough surface can be also produced by asymmetric deposition of oxide or nitride particles on implant surface. Currently we are studying the possibility of creating a rough surface by means of irregular and asymmetric deposition of particles on the smooth surface.
Particle distribution can be controlled for example by laser or electrical discharges. These particles then form granular surface that is well accepted by the body. Also in the case of surfaces prepared by this method may be reduced fatigue resistance of implant. Commonly realized surface finishes (for example machine parts with nitride smooth surface) are improving fatigue resistance [4]. The improvement of fatigue resistance is caused by high compressive residual stresses introduced within the diffusion zone [4]. Since such a layer hinders the dislocation motion, the predominant failure mechanism in the high cycle fatigue is subsurface crack growth. In case the granular surface, granules are relatively large and they could act as crack initiation sites. The size, scatter and depth of granules on surface must be appropriately designed in order to prevent this.

2. Theoretical model of fracture process
For the strain-deformation analysis of the behaviour of the granules in the surface is used 3D model based on the finite element method FEM. This model is based on the assumption that the granules are spheres partially embedded in the surface disposed on the surface as shown in figure 1. Model parameters (such as granules diameter, see figure 1, the diameter of granule is from 0.5 to 1mm and its height is 0.4 mm at maximum) can be easily changed in the program. The FEM model itself uses symmetry, so that the model represents only one quarter of the granules and the surrounding material. The model assumes that the crack forms at the interface between the granules and surrounding materials. The emergence of the crack is more likely if there is a sharp difference between the mechanical properties (for example elastic modulus) of the granules and the surrounding material. The mechanical properties of material surrounding the granules are exponential functions of distance from surface. For further analysis, model modification of model proposed Navarro [5,6] was utilized. Main advantage of this model is that definition of boundary length of crack is not needed for distinction between the initiation and propagation phases of crack growth.

The fracture mechanics is used for calculation of the number of cycles needed to propagate a crack to length of final rupture $a_{FR}$. The following equation expresses the number of cycles:

$$N \left( \sigma_{eq}, a \right) = N_{TR} \left( \sigma_{eq} \right) - \int_{a}^{a_{TR}} \frac{da}{C\Delta K^{m}}$$  \hspace{1cm} (1)

where $\sigma_{eq}$ is equivalent stress, $a$ length of crack and $N$ number of cycle. The constants $C$ and $m$ are known from Erdogan law. The subscript $TR$ means the total number of cycles to rupture. Limits of integral are $a$ – some crack length during fatigue process and $a_{FR}$ – the length at the time of the final rupture. Initiation phase of the fatigue process can be described by the integration of equation:

$$\frac{da}{dN} = C \left[ \Delta K^{m} - \Delta K_{th,Long} \left( \frac{a_{eq}^{p_{eq}}}{a_{eq}^{p_{eq}} + d_{eq}^{p_{eq}} - d_{eq}^{p_{eq}}} \right)^{\frac{p_{eq}}{2}} \right]$$  \hspace{1cm} (2)
Variables used in this equation are: \( AK_{th, Long} \) the growth threshold for long cracks; \( d_0 \) – the average distance to the first microstructural barrier; \( a_0 \) El Haddad parameter [7]. The \( P_{KT} \) factor is derived from the theoretical approximation of the Kitagawa–Takahashi diagram [8].

3. Specimens and the experimental procedure

3.1. Materials characterisation

Most of implants used in surgery are made from Ti-6Al-4V ELI alloy (Extra-Low Interstitials) currently. This alloy is very close to the alloy Ti-6Al-4V, which is intended for industrial use, but which may also arise in the construction of the implants. Ti-6Al-7Nb alloy or commercially pure titanium Grade 4 are being used as alternative materials. The surfaces studied in this work were made on specimens from these four titanium alloys. The mechanical properties of materials are shown in Table 1.

| Material                  | E [GPa] | \( \sigma_u \) [MPa] | \( \sigma_y \) [MPa] | \( \sigma_u,A \) [MPa] | \( \sigma_y,A \) [MPa] | C       | m      |
|---------------------------|---------|-----------------------|----------------------|-------------------------|-------------------------|---------|--------|
| Ti-6Al-4V ELI             | 113.8   | 893                   | 827                  | 998                     | 948                     | 7.9 \times 10^{-14} | 4.9     |
| Ti-6Al-4V                 | 117     | 944                   | 878                  | 1027                    | 978                     | 8.1 \times 10^{-14} | 5       |
| Ti-6Al-7Nb                | 105     | 920                   | 842                  | 1017                    | 983                     | 9.1 \times 10^{-14} | 4.8     |
| Pure Titanium             | 104.4   | 681                   | 552                  | 679                     | 549                     | 1.8 \times 10^{-14} | 5.13    |

Table 1. Mechanical properties: Young modulus \( E \), ultimate tensile strength \( \sigma_u \), yield stress \( \sigma_y \). The subscript \( A \) indicates the value after annealing of material. Constants \( C \) and \( m \) are known from Erdogan law. These constants were obtained for annealed titanium, if these constants are used the crack growth \( da/dN \) is \( m/cycle \) and value of stress intensity factor is MPa.m\(^{0.5}\).

Crack growth properties were measured according to ASTM E647.

In Figure 2 is marked HV hardness and its decline to \( 1/e \) and \( 1/2e \) of its value on the surface.

3.2. Surface treatment and surface layer

In the field of medical engineering, the most commonly surface treatment is deposition of TiO\(_2\). While nitridation has positive effect on the fatigue life of steels [4], it is not generally case of titanium alloys. In case of granular surfaces, the spots on the sample surface are heated and locally melted by electric arc or laser. Nitriding takes place virtually simultaneously with the formation of the granules on the surface. Plasma nitriding was used making TiN surface. The TiO\(_2\) surface was formed by two ways: Plasma Immersion Ion Implantation and Plasma spray. The TiO\(_2\) has other good properties such as self-cleaning [9]. Profiles of surface layers on granules of different surface layers with regions of possible crack initiation are displayed in figure 2. In this figure is marked HV hardness and its decline. Hardness of surface layer corresponds to content of oxide or nitride particles in diffusion zone.

4. Results and discussion

In Figure 3 is shown theoretical curves for all four types of titanium and for three types of surfaces. From the figure it is clear that the best results give Ti-6Al-4V ELI with TiO\(_2\) surface deployed by
Plasma Immersion Ion Implantation. This can be explained by the continuous distribution of particles on the granular surface. Worse outcomes for Plasma spraying method can be explained by presence of sharp transition, see figure 2. The worst results givenitridation of granuloid surfaces. The granules are throughout the volume nitride and between granules and smooth surface rise sharp transition stress.

Figure 3.
Experimental points: squares - Plasma Immersion Ion Implantation, triangles - Plasma spraying, circles- Nitriding; thick line - Ti-6Al-4V, dash thick line - Ti-6Al 4V ELI, thin line - Ti-6Al-7Nb, cash thin line - pure titanium.

5. Conclusion
The best results giveTi-6Al 4V ELI with granuloid TiO$_2$ surface, this can be explained by continuous transition of stress between granules and smooth surface.

Acknowledgments
This research has been supported by SPR No. 2124 of University of Hradec Kralove.

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