Optimization and Simulation of Residual Thermal Stresses Applied to 316 L Stainless Steel Biomaterial, Coated with a Layer of Titanium

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Abstract – In our study we performed the simulation of residual thermal stress generated at a titanium to stainless steel AISI 316L deposit using the Comsol Multiphysics 4.4 simulation software, the results obtained are compared with several manuscripts (theses, articles ...) that aim to treat vapor deposition (PVD) and the modeling and simulation of their results. To better approach of the experiment, it was assumed the stainless recessed substrate to replicate the effect of the sample holder and a cooling was imposed at a temperature of 20 ° C. The results obtained show that the titanium layer deposited is in high compression or its tendency to chipping after cooling.

Key words: residual thermal stress, Comsol Multiphysics 4.4, PVD, simulation, titanium, stainless steel

Introduction

The significant use of non-precious metal alloys in the field of biomaterials can be explained by their mechanical properties (hardness, high elastic limit, breaking strength), their ease of shaping (melting point, flowability) and their corrosion resistance in biological media. In this family of metals, it is mainly stainless steels, cobalt-based or nickel-based alloys enriched in chromium, molybdenum and titanium or titanium alloys [1]. The constituent materials of prosthesis are separated into three categories: support materials, ensuring mechanical fixation, friction materials ensuring the sliding of the articular surfaces and anchoring materials, ensuring the fixation of the prosthesis to the bone [1].Support materials are made up almost exclusively of metals, such as stainless steels [2]. Their main drawbacks are their toxicity and their plasticity. Titanium and its alloys based on aluminum and vanadium have many advantages: good biocompatibility, low plasticity and good fatigue resistance and especially low density [3,4]. The significant use of non-precious metal alloys in the field of biomaterials is explained by their mechanical properties, their ease of shaping, it is mainly stainless steels, cobalt-based or nickel-based alloys enriched in chromium, molybdenum and titanium or titanium alloys [1]. research has been carried out in order to be able to deposit thin layers (coatings), in particular titanium, on AISI 316L stainless steel using vapor deposition (PVD) techniques. Our work is to model and simulate this phenomenon of residual thermal stresses, in order to predict and control them during deposits

3 Simulations

To carry out the simulation we used the Comsol multiphysics 4.4 software, and the material is Stainless steel AISI 316L / (X2CrNiMo17-12-2) It is the most widely used metallic biomaterial, mainly in the field of orthopedic surgery, it has a carbon content of <0.03%.

4 Results

4.1. Total displacement

Figures (1) and (2) show the total displacement of our model, after cooling deposit at room temperature.

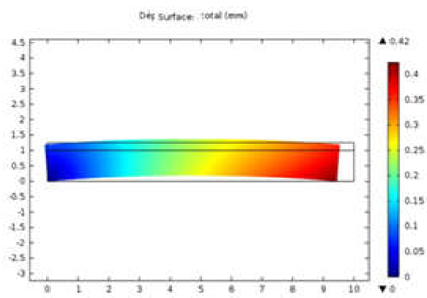

Figure1 2D model

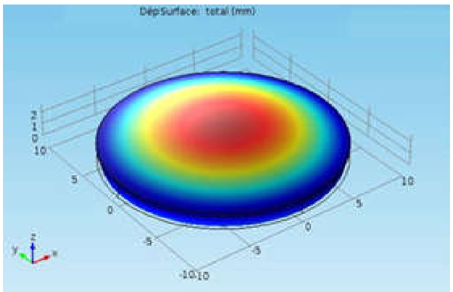

Figure 2 3D model

Overall we notice shrinkage of the coated plate, this is explained by the difference in the thermal expansion coefficients of the two layers (substrate / deposit), and this which causes the two layers to shrink differently. This difference in retraction is shown in the graph below:

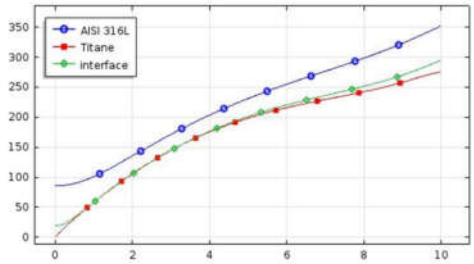

Figure2 differences in shrinkage of the two layers

From the graph, we see that the total displacement of the titanium coating has reaches 350 µm. While that of the substrate does not exceed 276µm, this confirms the idea that the two materials contract differently.Figure (4) shows the evolution of normal stresses along the cross section carried out through the two layers, we notice from the shape of this curve the increase in these stresses from -900 MPa at the bottom of the substrate to 1490 MPa at the top of this one. Approaching the interface, heat affected area where we notice a sudden drop in the value of internal stresses to -1400MPa. We explain this fall by the fact that, therefore the thermal stress is in compression in the deposit and in tension in the substrate. This result is comparable to those cited in theses [1] and [5].

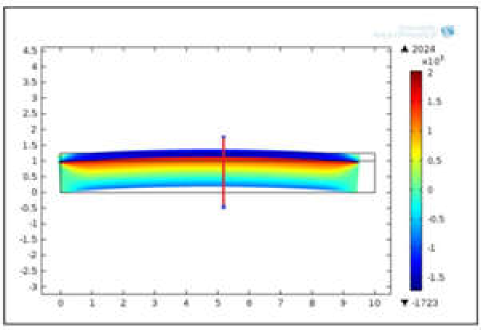

Figure 4 distributions of the residual stresses according to x in Mpa

1 Conclusion

The aim of this work was to simulate the residual thermal stresses, generated when depositing a thin layer of titanium on AISI316L stainless steel by the method PVD, our simulation allowed us to observe the following results:

- The part takes a convex shape after cooling, we can explain this result by the fact that the two layers shrink differently.

- Analysis of the distribution of residual thermal stresses in the two materials, allows us to conclude that they are due to the temperature gradient between the two materials during deposition and that their values are governed by the value of the thermal expansion coefficients of the two materials.

- The oxidation of titanium directly in contact with air gives TiO_2, which generates an important value of the Von stresses put therefore the exceeding of the limit locally to rupture hence the mechanism of scaling under high pressure. It can be concluded that the deposition of a thin layer of pure titanium on the substrate in AISI 316L stainless steel locally generates very high residual stresses that can cause breakage (chipping) of the material at scale local. These cracks can affect the life of parts in service.

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