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MATHEMATICAL MODELLING OF TECHNOLOGIES FOR THE DESIGN OF INNOVATIVE FUNCTIONAL BIO-COATINGS FOR DENTAL IMPLANTS

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ABSTRACT

The focus of this research is to determine a mathematical model for the bond strength of a discretely deposited nano-crystalline (DCD) hydroxyapatite (HAp) coating onto a dual acid-etched titanium dental implant. The research will focus on calculating the potential energy surface for the reaction of formation of a HAp coating to determine an activation energy for the reaction. This will give us the surface energy of the bonding of the HAp coating with titanium, or the bond strength of the coating.

Keywords: hydroxyapatite coating, bond strength, MD simulation.

INTRODUCTION

In previous studies it has been discovered that adding a new nano-scale HAp complexity to an already rough micro-topographical surface of a tooth implant (Figure 1) will result in a grafting response of the tooth on to the medical implant [e.g. [1], [2]). This will allow a faster recovery time for the patient and higher degree of reliability and stability of the implant for as long as it remains in the tooth. Since HAp can be crystalgraphically similar to bone mineral, and since the substance is bioactive and osteoconductive, when a discrete nano-scale layer of HAp is introduced to the micro-topography of the titanium implant, the increase in surface area and biocompatibility results in more space for upregulation of platelet activation and an increase in fibrin retention around the implant.

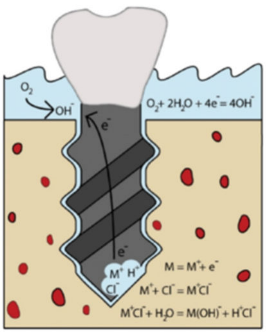

Fig. 1 - Chemical compatibility of implant (by Nejad, M. Kyle, S. 2017)

A biological matrix for osteogenic cell migration to the implant surface will be formed in response to this new increase in surface area and biological similarities of HAp nano-crystals [e.g. [3], [4]] (Figure 2).

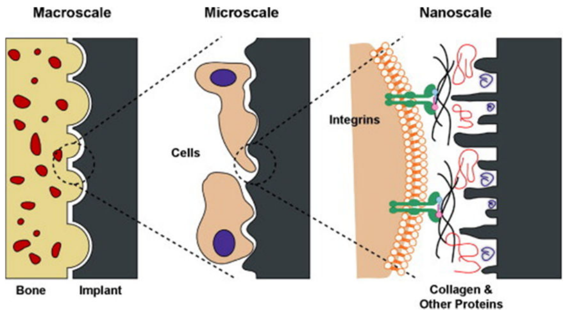

Fig. 2 - Suface topology (by Gittens, R. Olivares-Navarrete, R. *et al*. 2014)

In our Molecular Dynamic [e.g. [5]] simulations we will take into account both, crystallinity and nano-scale of the Hap coating (Figure 3).

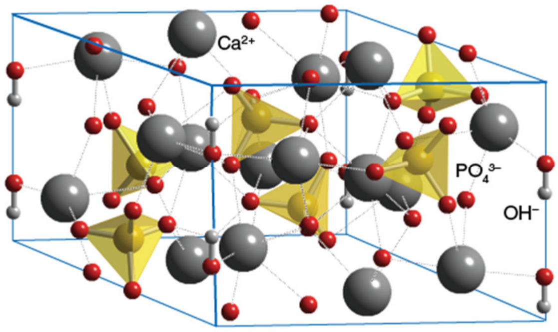

Fig. 3 - Current Bio-Active Coating (after Greeves, N. 2008)

There is a myriad of other advantages of an HAp DCD treated medical implant for bone healing, but perhaps understanding the substance HAp at its most fundamental physical and chemical conditions and calculating its strength will shed some light on further improvement of its applications and behavior in non-ideal environments.

REFERENCES

[1] Albrektsson, T., Johansson, C., “Osteoinduction, Osteoconduction, and Osteointegration”, European Spine Journal. Gottenburg, Sweden; pp. S96-S100 (2001).

[2] Durgalakshmi, D. Rakkesh, R.A. Balakumar, S., “Stacked Bioglass/TiO2, Nanocoatings on Titanium Substrate for Enhanced Osseointegration and its Electrochemical Corrosion Studies”, University of Madras, India, Applied Surface Science, Vol. 349; pp. 561-569 (2015).

[3] Gubbi, P., Towse, R., “Quantitative and Qualitative Characterization of Various Dental Implant Surfaces”, Biomet 3i.

[4] Hong, L. Wu, *et. al*., “Composite Coatings of 58S Bioglass and Hydroxyapatite on a Poly (Ethylene Terepthalate) Artificial Ligament Graft for the Graft Osseointegration in a Bone Tunnel”, Huashan Hospital Reearch Center of Biomedical Engineering, PRC. Applied Surface Science, Vol. 257; pp. 9371-9376 (2011).

[5] Balueva, A.V., Dashevskiy, I.N., “Atomistic Modeling and Strenth Calculations of Ni-Al Submicron and Nanosized Composites”, Proceedings “Recent Topics on Mechanics and Materials in Design”, M2D2017, Portugal, paper Ref: 6452; pp. 601-602 (2017).