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Multiscale Understanding of Biocell-Gold Adhesion

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ABSTRACT

With the advent of antibiotics and the concomitant advances in medical science, infectious diseases have become a much smaller health threat. On the other hand, as the average person's lifespan has increased, degenerative diseases have become critical issue in an aging population. More organs, joints, and other critical body parts wear out and need to be replaced. It is reported that biomaterial-associated infection was one of the most destructive complications occurring among the millions implants/replacements worldwide done in the late 20th century[1].

Current synthetic materials, such as stainless steel, titanium alloys, polymers, and ceramic composites expererience degradation after 10 to 15 years of use in the human body. Longer lives of patients may lead to several revision and replacement surgeries in their lifetimes[1,2]. A primary cause of failure is implant loosening by mechanical failure or poor biocompatibility between the materials and the body.[3] While the wear resistance of implant materials has improved, evaluating biocompatibility and quantify the adhesive strength of new materials remains a challenging task.

This work is to conduct multiscale computational simulations combined with experimental verification to evaluate the adhesive strength and thus biocompatibility at the interface between implant of different materials and bio-cells. Computational simulations includes Molecular Dynamics (MD) at the atom-nano scale, Finite Element Analysis (FEA) at the microscopic-cellular scale, and FEA at the macroscopic scale. Experimental approaches to verify simulation results include synthesizing biomaterials (biocomposite), cell culture, atomic force measurement, and microscopic fluid shear force measurement and high resolution electronic and nanoprobing techniques.

The objectives of this research is as follows:

Objective I: To understand the principles of interaction between the implant surface layer and fibroblast cells at the atom-nano scale and microscopic scale.

Objective II. To understand the adhesion mechanisms of implants and cells at macroscale.

Objective III. To develop methodology to bridge multi-scale simulation with experiments.

Our approach and results involve three length scales as follow:

- At the atom-nano scale
  The interface chemical composition of several kinds of synthesized biocomposites of implant is designed. Molecular dynamics (MD) calculations are conducted, the modeled interfacial bonding energy are then compared. This low-scale analysis will allow pre-selection of the chemical compositions with high adhesions. In addition, physical parameters such as viscosity and interfacing shearing force are assessed to consider the effect of chemical composition and the body fluid effect on these parameters. Our preliminary result shows that the implant with a gold surface layer covered on substrate shows relative high interfacial bonding energy compared to a bio-active ceramics material.

- At the microscopic (μm, single cell) scale
  Based on the measured basic surface geometric parameters and the MD-obtained physical parameters (e.g. viscosity), the FEA at the microscopic (μm) scale are conducted to obtain the corresponding maximum shear stresses. Comparing the calculated maximum shear stress with the measured shear strength by a rotating rheometer, the modified physical coefficient of the synthesized material and shear strength criterion are obtained, and thereafter, the coupled surface geometry-cell residency effects on the physical coefficient and strength criterion can be accounted for.

- At the macroscopic scale (>mm, multiple cells)
  The research work is still in the above two scales. After it is successful, the result will be used to design the interface morphology for the implant which include waviness, roughness, and porosity based on the measured basic surface geometry of the material coupon at the microscopic scale. FEA simulation, based on the confirmed physical coefficients, will be conducted to investigate the stress distribution with multiple cells in the model, and conduct a parametric study of asperities, waviness and porosities of the designed interface morphology on shear strength to optimize and enhance the interfacial adhesion.

REFERENCES

[1] K. M. Steven, The UHMWPE Handbook: "Ultra-High Molecular Weight Polyethylene in Total Joint Replacement", Elsevier Academic Press: San Diego (2004).

[2] Total Knee and Hip Arthroplasty, WebMD, April 21, 2007.

[3] M. C. Levesque, Arthintis: Knee Replacement Surgery, Am. Ac. Surg. (October 2006).