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MATHEMATICAL MODEL FOR SURFACE ENERGY MEASUREMENT DUE TO IMPLANT FAILURE IN TISSUE REPLACEMENT

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ABSTRACT

Even if metallic materials are available, it may be difficult to meet the expectations of young, active people following surgery. Revision surgery is needed when an implant fails for various reasons. Orthopaedic implant failure can result from aseptic loosening, metallosis, surgical or operational failure due to human or implanting machinery error, infectious failure in the periprosthetic joint due to poor hygiene maintenance during or after surgery, poor bone integration, and other mechanical mis Aseptic loosening caused 18% of implant failures due to Young's and bulk modulus incompatibilities. This causes considerable bone loss or osteolysis, slow wear and tear of the high-load bearing joint, stress-shielding effects, debris release that induces unfavourable cellular responses, osteoporosis, and implant failure. Nearly 20% of implant failures are infectious. Septic loosening inhibits implant function and produces pain and redness.

Keywords: Mathematical Model, Implant failure, Natural Tissue, Replacement.

1. INTRODUCTION

Despite the abundant availability of metallic materials in the market, fulfilling the expectations of youthful and dynamic persons post-surgery is very challenging. Revision surgery is required when an implant malfunctions for various reasons. Figure 1 illustrates that orthopedic implant failure may result from mechanical mismatches, including aseptic loosening, metallosis, surgical or operational errors attributable to human or machinery faults, infectious complications in the periprosthetic joint due to inadequate hygiene during or post-surgery, insufficient bone integration, among other factors. Aseptic loosening resulted in a discrepancy in mechanical parameters, including Young's modulus and bulk modulus, contributing to 18% of implant failures. It induces stress-shielding effects, progressive degradation of high-load bearing joints, the generation of debris that elicits adverse cellular responses, substantial bone loss or osteolysis, and ultimately osteoporosis and implant failure. Infection accounts for around 20% of implant failures. It induces septic loosening, resulting in pain, erythema, and suboptimal implant functionality (Heimann 2017; Quinn et al. 2020; Siddiqui et al. 2018; Kim et al. 2012; Lahiri et al. 2011b; Roy 2020).

Figure 1 The factors responsible for secondary surgery due to implant failure.

Titanium alloys' excellent toughness-to-mass ratio and corrosion resistance make them ideal for many critical applications. Titanium alloys are used in oil refinery heat exchangers and static and rotational gas turbine engine components. Titanium alloys are used in chemical processing, desalination, valve and pump components, and nautical equipment due to their corrosion resistance. Due of its high toughness-to-mass ratio, this alloy's components are lighter. The most prevalent titanium alloy is Ti-6A1-4V. However, Ti-6A1-4V alloy has poor wear and high-temperature surface properties. However, implantation seldom forms a connection with living bone, and implant integration into bone tissue takes months. Thus, accelerating osseointegration and reducing surgical limitations is of importance.

2. LITERATURE REVIEW

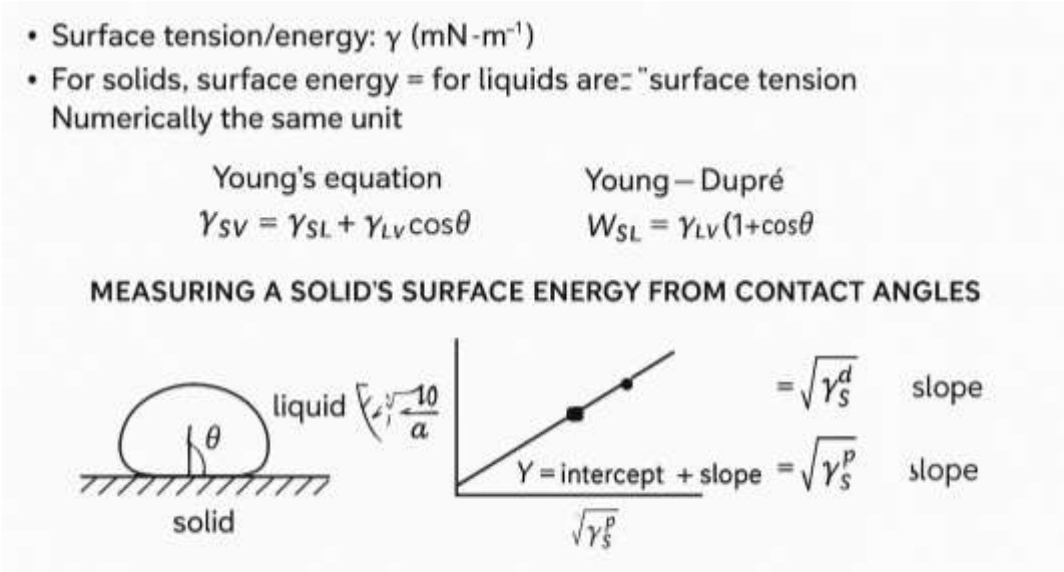
Steffi et al. (2018) suggested the manipulation of osteoclast interactions with orthopedic biomaterials to achieve an optimal balance between osteoclast resorption and osteoblast deposition for improved outcomes in orthopedic surgery implantation. The study examined how implant surfaces, bioceramics, and polymers influence osteoclast activity, considering factors such as topography, chemical composition, and surface modifications. Research indicates that coarser implant surfaces promote osteoclast activity, whereas smooth surfaces hinder differentiation. Alterations to the surface induced by anti-osteoporotic medication could enhance the integration of implants through a reduction in osteoclast activity. In vitro studies demonstrated that the characteristics of implant surfaces affect osteoclastogenesis, the activity of osteoclasts, and the process of bone remodeling.

The investigation revealed gaps in the existing literature, including studies on osteoblast activity that lack consideration of osteoclast differentiation. The authors suggested exploring the surface topography of implants, their chemical compositions, and the physiochemical effects on osteoclast activity. Future investigations may reveal that medications aimed at modulating osteoclast function enhance osteointegration. The findings suggest a potential enhancement in bone integration for orthopedic implants as time progresses (Steffi et al., 2018). Cadar et al. (2017) conducted an investigation into nanostructured and multisubstituted hydroxyapatite (HAp) incorporating Mg, Zn, Sr, and Si, focusing on its applications as orthopedic and dental bone replacement materials, along with its potential use in metallic implant coatings. Biomaterials were developed and characterized, with the release of Ca, P, Mg, Sr, and Si in water and SBF observed over a period of 1 to 90 days. The structure of the biomaterial and its interactions with water-SBF were confirmed through XRD and FTIR analysis. The evaluation of time-dependent element release was conducted using ICP-OES. Multisubstituted HAp materials generated physiological components at regulated rates, indicating their potential application in bone regeneration and as coatings to improve the biocompatibility and osteointegration of metallic implants.

The study did not address the inconsistencies in replacement limits and the challenges in reliably incorporating replacement components during material manufacture and characterization. The study focused on orthopedic and dental applications, thus excluding other medical applications or novel biomaterials for future investigation. Certain studies indicated a magnesium substitution of 2.46 wt% in hydroxyapatite, whereas other research suggested greater quantities. The theoretical limit for silicon phosphorus replacement is 5.8 wt%, but actual substitution typically ranges from 3-5 wt%. This underscores the necessity for further investigation to gain a deeper understanding of these limitations and their effects on material properties and performance (Cadar et al. 2017). Hydroxyapatite (HA) was explored as an orthopedic biomaterial due to its hemostatic and bone-regenerating properties, rather than using biocompatible and biodegradable bone wax. HA outperformed $CaSiO_3$, calcium-attapulgite, and calcium tripolyphosphate in terms of blood clotting activity, especially when adjustments were made for surface area and activity. Calcium ions The impact of synthetic HA on the blood clotting response was examined, as this response is essential for bone repair and integration, leading to an investigation of its effects on biological tissues. The hydrothermal synthesis of HA using $Ca(OH)_2$ and Na_2HPO_4 facilitated meticulous regulation of characteristics for ideal tissue compatibility.

Analysis of hemostatic polymers in relation to chitosan. Further investigation is necessary to gain a deeper insight into the impact of HA production on biological interactions and its effectiveness in hemostasis. Yang et al. (2017) suggest exploring the in vivo interactions of HA with biological systems to uncover its biodegradable and biocompatible properties for hemostatic bone healing. Hendrik et al. (2016) utilized accurate force field and pH-resolved surface models to simulate the chemical bonding, structural, surface, interfacial, and mechanical properties of hydroxyapatite (HA) grounded in experimental data. This force field has been utilized by AMBER, CHARMM, GROMACS, and other platforms to simulate apatite-biological systems with diverse compositions and ions. Surface models that account for pH variations offer improved approximations of interactions with apatite, particularly across diverse pH levels. The discussion focuses on the impact of HA on the mineralisation of bone and teeth. The quantitative monitoring of inorganic-biological assembly within the range of 1–100 nm enhances our comprehension of intricate biological-mineral interactions. Earlier models failed to accurately forecast the surface chemistry of HA, as well as its interfacial interactions, hydration, and protonation processes. This work addresses these concerns. The presence of these gaps hinders the advancement of research in bone and tooth mineralization. The findings indicate that existing models fail to accurately represent elevated OH-ion concentrations at the HA surface during hydration and protonation, along with physiologically rare pH levels exceeding 14. This constraint is essential for simulating solutions within biological systems. To enhance the accuracy of habitat recreation for living organisms, the authors suggest illustrating protonation effects on phosphate ions across different pH levels and employing more authentic solution conditions.

3. MATHEMATICAL MODEL FOR SURFACE ENERGY MEASUREMENT



3.1 One-component (dispersive only) approaches

(a) Fowkes (nonpolar liquids)

Assumes only dispersive forces:

$$W_{sl} = 2\sqrt{\gamma_s^d \gamma_l^d}$$

Combine with Young–Dupré:

$$\gamma_{lv}(1+\cos\theta) = 2\sqrt{\gamma_s^d \gamma_l^d} \Rightarrow \sqrt{\gamma_s^d} = \frac{\gamma_{lv}(1+\cos\theta)}{2\sqrt{\gamma_l^d}}$$

(b) Zisman plot (critical surface tension

Measure θ for a homologous series of liquids, plot $\cos\theta$ vs. γ_{lv}, and extrapolate to $\cos\theta = 1$. The intercept is γ_c, an empirical wetting threshold often close to—but not equal to—γ_s for low-energy, nonpolar solids.

3.2 Two-component (dispersive + polar)

Owens–Wendt–Rabel–Kaelble (OWRK)

Decompose into dispersive and polar parts:

$$\gamma_{lv}(1+\cos\theta) = 2\left(\sqrt{\gamma_s^d\gamma_l^d} + \sqrt{\gamma_s^p\gamma_l^p}\right)$$

Measure θ with ≥2 **liquids** of known (γ_l^d, γ_l^p). Solve the resulting linear system for (γ_s^d, γ_s^p). Then

$$\gamma_s = \gamma_s^d + \gamma_s^p.$$

Linearized form for regression with ≥3 liquids:

$$Y = \frac{\gamma_{lv}(1+\cos\theta)}{2\sqrt{\gamma_l^d}} = \sqrt{\gamma_s^d} + \sqrt{\gamma_s^p}\sqrt{\frac{\gamma_l^p}{\gamma_l^d}}$$

Fit Y vs. $X = \sqrt{\gamma_l^p/\gamma_l^d}$; intercept $= \sqrt{\gamma_s^d}$, slope $= \sqrt{\gamma_s^p}$.

3.3 Acid–base (Lewis) model
van Oss–Chaudhury–Good (vOCG)
Split into Lifshitz–van der Waals (dispersive) and acid–base components :

$$W_{sl} = 2\left(\sqrt{\gamma_s^{LW}\gamma_l^{LW}} + \sqrt{\gamma_s^+\gamma_l^-} + \sqrt{\gamma_s^-\gamma_l^+}\right)$$

With Young–Dupré:

$$\gamma_{lv}(1+\cos\theta) = 2\left(\sqrt{\gamma_s^{LW}\gamma_l^{LW}} + \sqrt{\gamma_s^+\gamma_l^-} + \sqrt{\gamma_s^-\gamma_l^+}\right)$$

Measure θ for ≥3 **liquids** of known $(\gamma_l^{LW}, \gamma_l^+, \gamma_l^-)$ and solve for $(\gamma_s^{LW}, \gamma_s^+, \gamma_s^-)$. The polar (acid–base) part is

$$\gamma_s^{AB} = 2\sqrt{\gamma_s^+\gamma_s^-}, \quad \gamma_s = \gamma_s^{LW} + \gamma_s^{AB}.$$

3.4 Component models — splitting surface energy

Most practical methods split total surface energy γ into components (typically **dispersive** and **polar**, sometimes acid/base):

$$\gamma = \gamma^d + \gamma^p$$

Common models below show how to estimate γ_S^d and γ_S^p using contact angles of two or more probe liquids with known component values.

4. RESULTS AND DISCUSSION

Materials introduced into the body must be handled carefully since they directly replace bodily components and bio-functions. As a result, there is no possibility of any infection from the biomaterial causing implant failure.

4.1. Mechanical Factors

- **Fatigue Failure**: Repetitive stress over time can lead to cracks or breakage in implants.
- **Wear and Tear**: Continuous articulation in joint replacements (e.g., hip or knee) can lead to debris generation and mechanical degradation.
- **Loosening or Dislocation**: Inadequate fixation, poor alignment, or patient activity can cause implants to loosen or migrate from the original site.
- **Stress Shielding**: Implants taking on too much load can lead to bone resorption due to reduced mechanical stimulation of surrounding bone tissue.

4.2. Biological Factors

- **Infection (Peri-implantitis or Biofilm Formation)**: Bacterial colonization of the implant surface can trigger chronic inflammation, leading to tissue damage and implant failure.
- **Immune Response or Allergic Reactions**: Host rejection or allergic response (e.g., to metal ions like nickel or cobalt) can compromise integration and function.
- **Poor Osseointegration**: Inadequate bone-implant bonding, especially in dental or orthopedic implants, leads to instability.

4.3. Material-Related Issues

- **Material Degradation**: Corrosion or oxidation of metallic implants, or degradation of polymeric materials, can compromise mechanical integrity and biocompatibility.
- **Inappropriate Material Selection**: Use of non-biocompatible or suboptimal materials can result in toxicity, immune responses, or mechanical failure.

4.4. Design and Manufacturing Defects

- **Improper Design Geometry**: May not accommodate stress distribution or biological integration effectively.
- **Manufacturing Defects**: Microcracks, surface irregularities, or poor finishing can initiate early failure.

Table 1 Multifunctional roles expected from biomaterial

Characteristics	Description
Augmentable	Ability to enhance or supplement the natural function of body parts
Anti-fungal	Resists or not serve as a sink for fungal development
Anti-fouling	Materials surface property to prevent bacterial attachment
Anti-corrosive	The material should resist corrosion in the biological environment
Bactericidal	An ability of a material to act and directly kill the pathogen
Bioactivity	Supportive response of the material to perform the biological functions of the tissues surrounded by it
Bioactive fixation	In the permanent implantation, a firm chemical and biological bond formation at the junction of material surface and tissue interface.
Bio-compatibility	Must not elicit an adverse response or reaction to surrounding tissue, compatible to blood, and be integral to the body environment
Biostability	The material ability to maintain its properties for a longer duration *in vivo*
Interfacial stability	The ability of the material to prevent surface mechanical failures under high load-bearing conditions

Characteristics	Description
Non-carcinogenic	Must not illicit carcinogenic material to form an inflammation or cancer
Nontoxic	Must not release toxic substances which harm the body environment
Nonpyrogenic	Materials should not elicit heat or fever when inserted into the body
Osseointegration	The ability of material in the enhancement of bone cell growth, which increases the interaction between the implant and surrounding tissue
Osteoconductive	The ability of a material to facilitate bone ingrowth through the surface of a biomaterial
Osteoinductive/ osteogenetic	Stimulating ability of a material to develop bone-forming cell lineage into the material the process also referred to as osteogenesis
Resorpability	Support gradual degradation over time to be replaced by the natural tissue
Sterilisable	Capable of undergoing sterilization to kill microbe if present by a different technique like dry heat, autoclave, ethylene oxidation, radiation, without losing its original property
Therapeutic capable agent	Supportive for drug delivery and growth factors at required times
Wettability	The material tendency of adherence/repulsion with the water molecules.
Wear-resistant	In bone joint replacement, the material should resist friction and not elicit wear particle into the body

Despite the therapeutic effectiveness of HA coatings, their brittleness results in worse mechanical and tribological qualities. Particularly poor surface mechanical qualities, such as low fracture toughness, bending strength, bonding strength, tensile strength, and wear resistance. Furthermore, HA-modified biomaterial surfaces are prone to bacterial colonization. As a result, researchers in this field will confront several problems and possibilities when creating HA composite coatings in order to achieve required qualities and overcome HA coating shortcomings.

4.5 Raman Spectroscopy

Raman spectroscopy is more sensitive in detecting minute phase changes(Ferrer et al. 2010). It provides more valuable insights into the material's amorphous and crystalline nature of coatings(Sergo et al. 1997).The powder and coatings were exposed to laser source emitting at 526nm wavelength, 10mW laser power for 10s of acquisition time in compact raman spectrometer (Renishaw, United Kingdom equipment).

5. CONCLUSIONS

Secondary operations often result from surgical, biological, mechanical, and patient-specific factors. Reduce implant failure via careful material selection, surgical planning, patient screening, and postoperative care. Emerging technologies include bioactive coatings, smart implants with sensors, and customizable 3D-printed implants reduce these difficulties. These biomaterials are selected for biocompatibility, degradability, mechanical strength, and bioactivity. Ceramics and bioactive glasses promote bone ingrowth; metals and alloys provide load bearing durability; composites synergize multiple properties; hydrogels recreate soft tissue environments and enable drug/cell delivery; and decellularized matrices retain native architecture and biological cues to guide rege

REFERENCES

1. Siddiqui, H., Pickering, K., and Mucalo, M. (2018). “A Review on the Use of Hydroxyapatite-Carbonaceous Structure Composites in Bone Replacement Materials for Strengthening Purposes.” *Materials (Basel).*, 11(10), 1813.

2. Spriano, S., Yamaguchi, S., Baino, F., and Ferraris, S. (2018). “A critical review of multifunctional titanium surfaces: New frontiers for improving osseointegration and host response, avoiding bacteria contamination.” *Acta Biomater.*, 79, 1–22.

3. Steffi, C., Shi, Z., Kong, C., and Wang, W. (2018). “Modulation of Osteoclast Interactions with Orthopaedic Biomaterials.” *J. Funct. Biomater.*, 9(1), 18.

4. Stewart, C., Akhavan, B., Wise, S. G., and Bilek, M. M. M. (2019). “A review of biomimetic surface functionalization for bone-integrating orthopedic implants: Mechanisms, current approaches, and future directions.” *Prog. Mater. Sci.*, 106(March), 100588.

5. Sun, L. (2018). “Thermal Spray Coatings on Orthopedic Devices: When and How the FDA Reviews Your Coatings.” *J. Therm. Spray Technol.*, Springer New York LLC.

6. Sun, L., Berndt, C. C., Gross, K. A., and Kucuk, A. (2001). “Material fundamentals and clinical performance of plasma-sprayed hydroxyapatite coatings: A review.” *J. Biomed. Mater. Res.*, 58(5), 570–592.

7. Surmenev, R. A., and Surmeneva, M. A. (2019). “A critical review of decades of research on calcium

phosphate–based coatings: How far are we from their widespread clinical application?” *Curr. Opin. Biomed. Eng.*, 10, 35–44.
8. Tercero, J. E., Namin, S., Lahiri, D., Balani, K., Tsoukias, N., and Agarwal, A. (2009). “Effect of carbon nanotube and aluminum oxide addition on plasma-sprayed hydroxyapatite coating’s mechanical properties and biocompatibility.” *Mater. Sci. Eng. C*, 29(7), 2195–2202.
9. Vu, A. A., Robertson, S. F., Ke, D., Bandyopadhyay, A., and Bose, S. (2019). “Mechanical and biological properties of ZnO, SiO2, and Ag2O doped plasma sprayed hydroxyapatite coating for orthopaedic and dental applications.” *Acta Biomater.*, 92, 325–335.
10. Vukelić, M., Mitić, Ž., Miljković, M., Živković, J., Ignjatović, N., Uskoković, D., Vasiljević, P., Petković, M., Živanov-Čurlis, J., and Najman, S. (2011). “interaction of biomaterials containing calcium hydroxyapatite/poly-l-lactide with the simulated body fluid.” *Acta medica Median.*, NA(NA), 35–39.
11. Wang, M. (2003). “Developing bioactive composite materials for tissue replacement.” *Biomaterials*, 24(13), 2133–2151.
12. Weiner, S., and Traub, W. (1992). “Bone structure: from ångstroms to microns.” *FASEB J.*, 6(3), 879–885.
13. White, A. A., Best, S. M., and Kinloch, I. A. (2007). “Hydroxyapatite-Carbon Nanotube Composites for Biomedical Applications: A Review.” *Int. J. Appl. Ceram. Technol.*, 4(1), 1–13.
14. William D. Callister, J. D. G. R. (2014). *Materials science and engineering: an introduction*. *John Wiley Sons, Inc.*, (9th Edition, ed.).
15. Yang, J., Cui, F., Seop, I., and Wang, X. (2010). “Plasma surface modification of magnesium alloy for biomedical application.” *Surf. Coat. Technol.*, 205, S182–S187.
16. Yang, Y., Zhou, H., Ni, X., Yang, M., Hou, S., Bi, Y., and Deng, L. (2017). “Hydroxyapatite: a promising hemostatic component in orthopaedic applications.” *Biol. Eng. Med.*, 2(1), NA-NA.
17. Zhou, X., and Mohanty, P. (2012). “Electrochemical behavior of cold sprayed hydroxyapatite/titanium composite in Hanks’ solution.” *Electrochim. Acta*, 65, 134–140.