

COMPUTATIONAL MODELING OF BIODEGRADATION OF METALLIC BIOMATERIALS

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1. INTRODUCTION

From a biodegradation perspective, biomaterials can be classified into two categories: bio-inert and biodegradable. Although bio-inert biomaterials show a great performance especially in fixation applications, they bring an important problem into the play: they remain in the body forever or require additional surgery to remove them. Biodegradable materials do not have this problem, and in the case of metallic biomaterials, they also provide a dynamic (i.e. time-varying) mechanical stability profile. However, taking advantage of them requires tuning the degradation parameters and material release rate.

Developing a quantitative mathematical model of the degradation process is a possible solution to this issue as it allows researchers to study the biodegradation behavior of any desired metallic scaffold or implant in-silico (in the computer) prior to conducting any in-vitro or in-vivo experiments.

2. MATERIALS AND METHODS

In this study, we have developed a quantitative mathematical model to predict the biodegradation of metallic biomaterials. Magnesium (Mg) has been selected to start with due to its acceptable mechanical properties, biocompatibility, and contribution in osteoinductivity [1]. The developed model captures the release of Mg ions, the formation of a protective film, and the dissolution of this film due to the effect of Chloride ions in the surrounding fluid. This has been accomplished by deriving a system of nonlinear time-dependent reaction-diffusion partial differential equations from the underlying oxidation-reduction reactions. The Level Set formalism has been employed to track the biodegradation interface between the biomaterial and its surroundings. The equations were solved implicitly using the finite element method on an adaptive mesh. The developed

model required calibration, which has been accomplished by implementing a Bayesian optimization algorithm and performing parameter estimation using the immersion tests data of the Mei et al. work [2].

3. RESULTS AND DISCUSSION

Figure 1 shows the comparison of the degraded shape of a screw (white body) with its initial shape (transparent surface). The color contour shows the release of Mg²⁺ to the cylindrical medium.



Fig 1. Simulation result of Mg²⁺ ions release (ion concentration in g/mm³) and biodegradation of a simple screw

The current model can be used as an important tool to find the appropriate design and degradation properties of the metallic implants for different biomedical applications. In the next step, the model will be also extended to include the biodegradation behavior of Iron and Zinc.

References

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