High-performance simulation of biodegradation behavior of magnesium-based biomaterials

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ABSTRACT

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 case of metallic biomaterials, they also provide a dynamic (i.e. time-varying) mechanical stability profile, but taking advantage of them requires tuning the degradation parameters and material release rate.

Developing a quantitative mathematical model of the degradation process is a proper solution to this issue by allowing researchers to study the biodegradation behavior of any desired implant in-silico (in the computer) prior to conducting any in-vitro or in-vivo experiments. Developed mathematical models can be simulated using efficient numerical schemes such as the finite element method. The primary challenge here will be achieving a high accuracy at the interface between the implant and surrounding tissue in the body as the interface plays an important role in the degradation phenomena. Increased accuracy means increased computational cost and resources (especially time), but high-performance computing (HPC) techniques can be used to overcome this challenge.

In this study, we have developed a quantitative mathematical model to predict the biodegradation of magnesium-based implants. 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 PDEs from the underlying oxidation-reduction reactions. The Level Set formalism has been employed to track the biodegradation interface between the implant and its surroundings. The equations were solved implicitly using the finite element method for spatial terms (with a 1^{st} order Lagrange polynomial as the shape function) and backward-Euler finite difference method for temporal terms on an Eulerian mesh. The mesh has been refined adaptively on the interface to increase the numerical accuracy of the simulated model. In order to increase performance and efficiency, the code has been developed in a way that can be distributed across several computational nodes. The code is implemented in FreeFem++ [2] and uses Message Passing Interface (MPI) to parallelize numerical integration on the investigated mesh. It also uses MUMPS distributed solver to solve the derived system of algebraic equations. A typical 3D biodegradation simulation usually consists of 600,000 elements and a DOF of 400,000, approximately.

Currently, the model has been validated with experimental data and simple scaffold shapes, so it can be used as an important tool to find the appropriate design and degradation properties of the magnesium-based implants for different biomedical applications. In the future, the model will be also extended to include the biodegradation behavior of Iron and Zinc.

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REFERENCES

[1] S. Agarwal et al (2016) Biodegradable magnesium alloys for orthopedic applications: A review on corrosion, biocompatibility and surface modifications. Mater Sci Eng C 68: 948-963.

[2] F. Hecht (2012) New development in FreeFem++. J Numer Math 20:251–265