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Simulation of the Change in Mechanical Properties of Degradable Bone Implants

Ann-Kathrin Krüger[1]*, Stefan Julmi[2], Christian Klose[2], Silke Besdo[1] and Peter Wriggers[1]

Micro Abstract
To develop and scale degradable bone implants, it is necessary to know the change in mechanical properties of the implant during the degradation process. In this study magnesium sponge structures are being investigated. It is assumed that the magnesium degradation is governed by diffusion of magnesium ions from the surface. To simulate the degradation a numerical model including the diffusion equation was developed. The model was implemented in the commercial finite element code Abaqus/Standard.

[1]Institute of Continuum Mechanics, Leibniz Universität Hannover, Hannover, Germany
[2]Institut für Werkstoffkunde, Leibniz Universität Hannover, Garbsen, Germany
***Corresponding author**: krueger@ikm.uni-hannover.de

Introduction

In consequence of diseases or accidents, bone tissue has to be removed or can be destroyed. This results in defects in the tissue. Defects of a size which the body cannot fill autonomously are called critical size defects (CSDs). CSDs indicate the use of a bone graft or an implant [8]. Bone grafts can be autogenic (from the patient himself), allogenic (from another human being) or xenogenous (from an animal). It is common to use autogenic grafts, but this means an additional surgery for the patient. Allogenic and xenogenic bone grafts can lead to infections and the risk of transmission of diseases is high [7]. To reduce the costs and the risk for the patient, artificial bone replacement materials are developed. For the application as implants, magnesium alloys turned out to be a promising solution in regards to their highly biocompatibility, good mechanical properties and controllable degradation behaviour. In previous studies different implant structures and different magnesium alloys have been investigated regarding their biocompatibility and degradation behaviour [5]. Open pored sponge like structures have been developed and investigated as bone tissue can grow into these structures [3]. Combining these features, the bone can grow into the implant, bridge the gap and the implant degrades as the bone grows.

1 Degradation model

To get a better understanding of the change in mechanical properties of the implant during the degradation process, a degradation model was developed. The knowledge about the mechanical properties of the degraded implant is essential for the development of such implants for different applications. The degradation model is build on a fortran code and the finite element code Abaqus/Standard.

1.1 Principles

The degradation model, developed in this study, is based on the behaviour of the magnesium alloy LAE442. Previous studies showed no significant change in volume of LAE442-implants during the implantation time coincident with a reduction of the implant stiffness [6]. Concurrently the formation of a degradation layer was recognizable and magnesium ions were detected in the environment of the implant [4]. The degradation layer shows a change in material composition compared to the base material [4], and thus results in a change of mechanical properties of the implant. It is assumed in this study that the magnesium degradation is dominated by diffusion of magnesium ions from the surface. To simulate the degradation a numerical model including the diffusion equation was developed [1].

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{1}$$

D is the diffusion coefficient and c is the magnesium concentration. The simulation model is based on the assumption that the Young's modulus (E) of the material depends on the magnesium concentration

$$E(c) = \frac{c}{c_0}E_0 \tag{2}$$

and that the magnesium concentration decreases from the surface to the material core gradually. Additionally, the magnesium concentration at the surface of the implant decreases, related to the flux of magnesium ions and the mass transfer coefficient of the environment [1].

$$-D\frac{\partial c}{\partial t} = \beta(c - c_{env}) \tag{3}$$

Herein β is the mass transfer coefficient and c_{env} is the magnesium concentration in the environment. In this case of implants the environment mainly consists of blood.

The formation of the degradation layer was realised by dividing the domain into the not-degraded magnesium core and the degradation layer. Figure 1 shows the assumed magnesium concentration through a bar of the sponge structure for two different degradation layer thicknesses, d_i. The dark grey area is the magnesium core, while the lighter grey areas represents two different degradation layers. The concentration in the magnesium core is assumed to have a constant value, c_{MG}, while the concentration in the corrosion layer and the environment decreases from inside to outside. The concentration far from the surface is supposed to have a constant value too, c_{Env}.

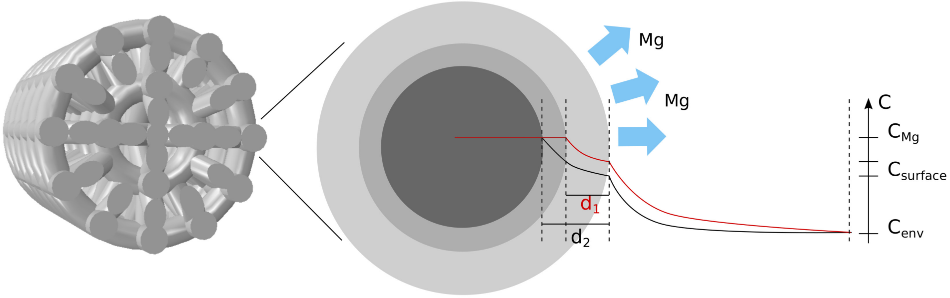

Figure 1. Assumed magnesium concentration through a bar of the sponge structure.

1.2 Computation

The computation of the chemical and mechanical part of the degradation model is sequentially-coupled. Accordingly, the diffusion analysis and the static analysis are seperated, but the static analysis is dependent on the results of the diffusion analysis. To compute the magnesium concentration field for different degradation layer thicknesses, the domain is divided into two regions, see Figure 1, using a signed distance field. The division takes place at the node level, in order to get at most a mesh-independent solution. For every node of the domain, the magnesium concentration was computed during an Abaqus diffusion analysis. For the mechanical part of the model, compression tests with the degraded structure were simulated to calculate the effective Young's modulus of the structure for different degradation layer thicknesses. Therefore, the concentration field from the diffusion analysis was transfered and an Abaqus static analysis with the concentration-dependent Young's modulus was executed.

2 Results

During the degradation the magnesium content decreases from the core to the surface. In Figure 2a, the magnesium distribution with a degradation layer thickness of 0.14 mm is demonstrated. The red area represents the magnesium core with the initial magnesium concentration. Figure 2b shows the experimental result of a structure, made of the LAE442 alloy, after 2 weeks in simulated body fluid (SBF). The bright area is the undegraded magnesium. The degradation layer has been removed by an acid treatment in chromic acid. Comparing the red and the bright area there are similarities in the shape and the degradation behaviour, like the rounding of the pores.

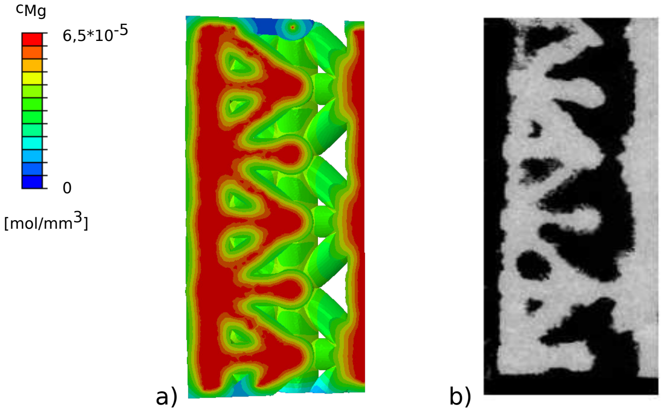

Figure 2. a) Magnesium concentration field of the sponge structure with a degradation layer thickness of 0.14 mm. b) CT-image of a sponge structure after 2 weeks in simulated body fluid.

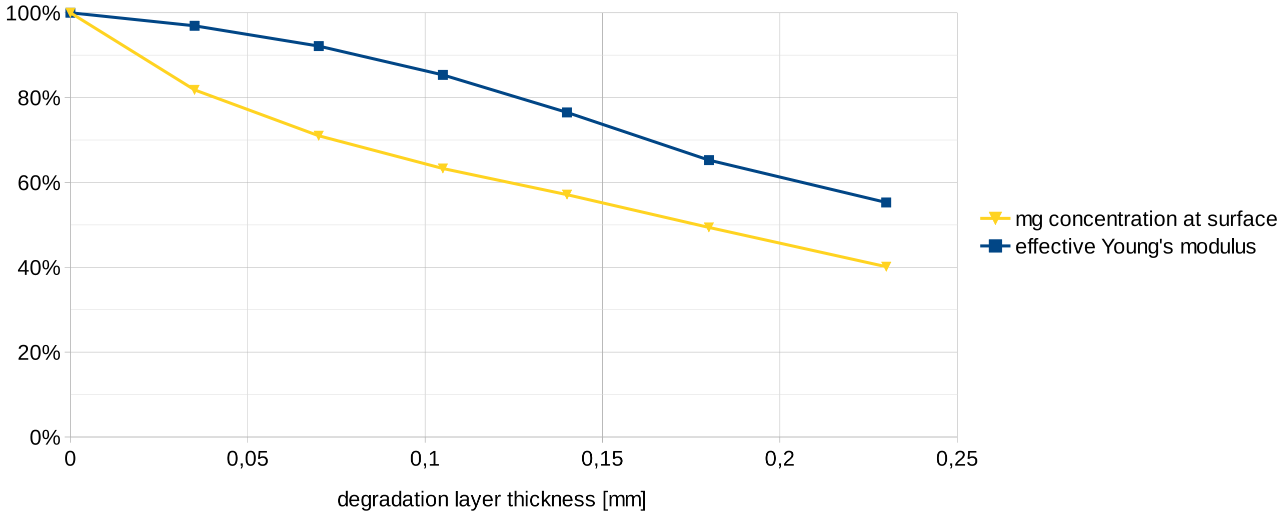

Figure 3. Yellow graph) Decrease of the magnesium concentration at the surface with increasing degradation layer thickness. Blue graph) Decrease of the effective Young's modulus with increasing degradation layer thickness.

By increasing of the degradation layer, the magnesium concentration at the surface, as well as the effective Young's modulus decreases, see Figure 3. Since the diameter of the bars of the sponge structure is 0,5 mm, the structure is totaly degraded if the thickness of the degradation layer is 0,25 mm. If the degradation layer has a thickness of 0,23 mm there is nearly no magnesium core left. The effective Young's modulus of the structure decreases to 55 % of the inital value. The concentration at the surface decreases to 40 % of the initial value.

Conclusion

With the simulation model, the formation of the degradation layer is computable, as well as the change in mechanical properties, as measured by the effective Young's modulus of the structure. Additionally, first comparisons with experimental results show similarities. There are a number of studies, which are concerned with the corrosion of magnesium. For instance, the work from Grogan et al., who developed a physical corrosion model [2]. But this is the first approach to model the formation of the degradation layer in combination with a mechanical analysis. However, the model is time-independent yet. For a better understanding of the degradation process, the model has to be time-dependent. As a result, the relationship between the degradation layer thickness and the degradation time has to be investigated further by extending the model by the interface between the magnesium core and the degradation layer.

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References

[1] H. D. Baehr and K. Stephan. *Heat and Mass Transfer.* Springer-Verlag, Berlin Heidelberg, 2011.

[2] J. A. Grogan, S. B. Leen, and P. E. McHugh. A physical corrosion model for bioabsorbable metal stents. *Acta Biomaterialia*, Vol. 10:p. 2313–2322, 2014.

[3] S. Julmi, C. Klose, A.-K. Krüger, P. Wriggers, and H. J. Maier. Development of sponge structure and casting conditions for absorbable magnesium bone implants. In *TMS 2017: Proceedings of the 146th Annual Meeting & Exhibition Supplemental, February 26-March 2, San Diego, California, USA.*, pages 307–317, City, 2017. Publisher.

[4] A. Kraus. *Untersuchung der Degradation und Biokompatibilität von degradablen, intramedullären Implantaten auf Magnesiumbasis im Kaninchenmodell.* Tierärztliche Hochschule Hannover, Dissertation, 2008.

[5] J. Reifenrath, D. Bormann, and A. Meyer-Lindenberg. Magnesium alloys as promising degradable implant materials in orthopaedic research. In *Magnesium Alloys - Corrosion and Surface Treatments.* Frank Cerwinski(Ed.), InTech, DOI: 10.5772/14143, 2011.

[6] C. Rössig, N. Angrisani, P. Helmeck, S. Besdo, J.-M. Seitz, B. Welke, N. Fedchenko, H. Kock, and J. Reifenrath. In vivo evaluation of a magnesium-based degradable intramedullary nailing system in a sheep model. *Acta Biomaterialia*, Vol. 25:p. 369–383, 2015.

[7] H. Sailer and F. Weber. Knochenersatzmaterialien. *Mund Kiefer Gesichts Chir*, Vol. 4:p. 384–391, 2000.

[8] J. P. Schmitz and J. O. Hollinger. The critical size defect as an experimental model for craniomandibulofacial nonunions. *Clin Orthop Res.*, Vol. 205:p. 299–308, 1986.