An IGA approach to chemo-electro-mechanical coupling in flexoelectricity-induced bone remodelling

Andreas Menzel[1,2], Carina Witt[1] and Tobias Kaiser[1]

[1]Institute of Mechanics, Department of Mechanical Engineering, TU Dortmund University, Leonhard-Euler-Str. 5, D-44227 Dortmund, Germany
andreas.menzel@udo.edu, carina.witt@tu-dortmund.de, tobias.kaiser@tu-dortmund.de

[2]Division of Solid Mechanics, Lund University, P.O. Box 118, SE-221 00 Lund, Sweden
andreas.menzel@solid.lth.se

The effect of flexoelectricity, which couples strain gradients with electric polarisation in a broad range of materials, see e.g. [1], has recently been found to be present in cortical bone and, in particular, to play a role in bone remodelling processes. More specifically, Núñez-Toldrà et al. [2] experimentally showed that flexoelectricity can induce osteocyte apoptosis in mechanically stimulated bones which is a starting point for targeted bone remodelling. Due to the size-dependency of flexoelectricity, the importance of this effect is most relevant on small scales. Accordingly, strain gradients in the vicinity of bone micro cracks lead to the generation of electric fields that are sufficiently high to induce osteocyte apoptosis.

Since successful bone remodelling is most relevant to maintain the structural integrity of bones, it is crucial to investigate the entire process, starting with the initiation by, e.g., flexoelectricity and proceeding with bone cell migration and formation of new bone material. However, appropriate experiments are difficult to conduct and consequently, a computational modelling approach has been proposed in [3] which can be used to study the process by numerical simulations.

Due to the higher gradients that occur in the governing equations when flexoelectricity is considered, Isogeometric Analysis [4] is employed in this computational approach since the NURBS basis functions used therein possess the required continuity properties. Apart from the electro-mechanical coupling in terms of flexoelectricity, a coupling to chemical fields is employed in order to model the behaviour of the different bone cells and biochemical signals which participate in the remodelling process. The involved bone cells in this regard are osteocytes, osteoclasts and osteoblasts, whereas the signalling tasks are performed by different types of messenger substances in the proposed model. All of these chemical substances and bone cells are accounted for by the introduction of additional field variables as well as diffusion equations so that a chemo-electro-mechanical coupling is obtained.

The proposed modelling approach is applied to the initial boundary value problem of a small sample of cortical bone with a narrow micro crack subjected to a mechanical tensile load. In this example, particular focus is on the electric fields that are induced in consequence of the flexoelectric effect, as well as on the subsequent cell diffusion which leads to remodelling.

[1] Shu, L., Liang, R., Rao, Z., Fei, L., Ke, S., Wang, Y. Flexoelectric materials and their related applications: A focused review. J. Adv. Ceram. 8, 153173, 2019, https://doi.org/10.1007/s40145-018-0311-3

[2] Núñez-Toldrà, R., Vasquez-Sancho, F., Barroca, N., Catalan, G. Investigation of the cellular response to bone fractures: Evidence for flexoelectricity. Sci. Rep. 10, 254, 2020, https://doi.org/10.1038/s41598-019-57121-3

[3] Witt, C., Kaiser, T., Menzel, A., Modelling and numerical simulation of remodelling processes in cortical bone: An IGA approach to flexoelectricity-induced osteocyte apoptosis and subsequent bone cell diffusion. J. Mech. Phys. Solids, 173, 105194, 2023, https://doi.org/10.1016/j.jmps.2022.105194

[4] Cottrell, J.A., Hughes, T.J.R., Bazilevs, Y. Isogeometric Analysis: Toward Integration of CAD and FEA. Wiley, Chichester, 2009