11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

MULTISCALE ELASTOPLASTICITY OF POROUS POLYCRYSTALS: FUNDAMENTALS AND APPLICATION TO OSTEONAL FAILURE IN LAMELLAR BONE

Claire Morin[1,2], Viktoria Vass[1] and Christian Hellmich[1]

[1] Institute for Mechanics of Materials and Structures, Vienna University of Technology (TU Wien), 1040 Vienna, Austria; Viktoria.Vass@tuwien.ac.at, Christian.Hellmich@tuwien.ac.at

[2] Ecole Nationale Supérieure des Mines, CIS-EMSE, CNRS:UMR5146, LGF, F-42023 Saint-Etienne, France; claire.morin@emse.fr

Key Words: *Osteon push-out, non-linear micromechanics, multisurface plasticity*

Mechanical modeling of porous polycrystals may pose considerable challenges: Classical two-phase self-consistent schemes [8] cannot capture the mechanical behavior of high-porosity materials, while discretization of each and every single crystal by finite elements may require disproportionate efforts in terms of CPU, or may be even impossible due to restricted access to the required microstructural details. As a recent remedy, continuum micromechanics formulations were extended as to involve an infinite number of non-spherical crystal phases, interacting with a spherical pore phase [4,5], see also Figure 1. Such formulations allow for satisfactory predictions of the (poro-)elasticity and brittle strength of vast classes of porous polycrystals (such as hydroxyapatite, bioactive glass-ceramics, gypsum, alumina, or zirconia), [7]. Additional physical phenomena appear if the polycrystals are hydrated. Then, probably sliding events along very thin (liquid crystalline) water layers forming interfaces between or within the single crystal phases entail ideal plastic behavior of crystals (or clusters thereof). Its occurrence in the extrafibrillar space of bone ultrastructure, together with brittle rupture of collagen, could well explain the strength of different bone samples from different species, ages, and anatomical locations [6]. This explanation, however, required major micromechanical developments, which we refine and extend in the present contribution: The sliding-related elastic-perfectly plastic constitutive law [4] is elaborated for a non-associated Mohr-Coulomb plasticity. Upscaling this elastoplastic behavior from the single crystal to the polycrystal scale is achieved through derivation of concentration and influence tensors for eigenstressed microheterogeneous materials [11], which itself is a generalization of the well-known transformation field analysis [3]. The the resulting multiscale-multisurface elastoplasticity problema is solved through a new variant of the algorithmic strategy of “return-mapping” [12].

We here focus on microscopic strength properties as determined through pushing osteons out of pieces of Haversian lamellar bone [1]. Such tests produce an almost pure shear (micro-)stress state at the outer boundaries of the osteons. These boundaries are called cement lines, and they are characterized by a very low collagen content [2], so that the RVE depicted in Figure 1 turns out as relevant for the cement line material. The volume fractions of crystals and pores inside this polycrystalline RVE follow universal composition rules valid for all bone tissues, and described in more detail in [10] and references therein. Ultimate loads bearable by osteons under punching loads as predicted by the newly developed multiscale-multisurface elastoplastic model agree very well with corresponding experiments [1].

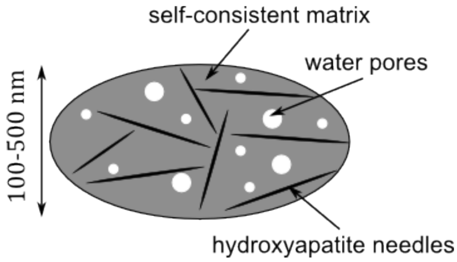

Figure 1: RVE of porous polycrystal, as found in the extrafibrillar space of bone.

To our best knowledge, this is a true *premiere* in both multiscale elastoplasticity and bone mechanics, and holds the promise for significantly improved computer-aided fracture risk assessment in orthopedics.

REFERENCES

[1] R. F. Bigley et al. Osteon interfacial strength and histomorphometry of equine cortical bone. *Journal of Biomechanics*, Vol. **39**, pp. 1629-1640, 2006.

[2] D.B Burr et al. Composition of the cement line and its possible mechanical role as a local interface in human compact bone. *Journal of Biomechanics*, Vol. **21**, pp. 939–945, 1988.

[3] G. J. Dvorak and Y. Benveniste. On Transformation Strains and Uniform Fields in Multiphase Elastic Media. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, Vol. **437**, pp. 291–310, 1992.

[4] A. Fritsch et al. Mechanical behavior of hydroxyapatite biomaterials: An experimentally validated micromechanical model for elasticity and strength. *Journal of Biomedical Materials Research Part A*, Vol. **88A** (1), pp. 149–161, 2009.

[5] A. Fritsch, L. Dormieux and C. Hellmich. Porous polycrystals built up by uniformly and axisymmetrically oriented needles: homogenization of elastic properties. *Comptes Rendus Mécanique.* Vol. **334**, pp. 151–157, 2006.

[6] A. Fritsch, C. Hellmich and L. Dormieux, Ductile sliding between mineral crystals followed by rupture of collagen crosslinks: Experimentally supported micromechanical explanation of bone strength. *Journal of Theoretical Biology*, Vol. **260**, pp. 230–252. 2009.

[7] A. Fritsch, C. Hellmich and P. Young. Micromechanics-Derived Scaling Relations for Poroelasticity and Strength of Brittle Porous Polycrystals. *Journal of Applied Mechanics*. Vol. **80** / 020905-1, 2013.

[8] R. Hill. A self-consistent mechanics of composite materials. *Journal of the Mechanics and Physics of Solids*, Vol. **13**, pp. 213-222, 1965.

[9] R. N. McCarthy, L. B. Jeffcott and R. N. McCartney. Ultrasound speed in equine cortical bone: effects of orientation, density, porosity and temperature. *Journal of Biomechanics*, Vol. **23**, No. 11, pp. 1149-1143, 1990.

[10] C. Morin and C. Hellmich. Mineralization-driven bone tissue evolution follows from fluid-to-solid phase transformations in closed thermodynamic systems. *Journal of Theoretical Biology.* Vol. **335**, pp. 185-197, 2013.

[11] B. Pichler and C. Hellmich. Estimation of Influence Tensors for Eigen- stressed Multiphase Elastic Media with Nonaligned Inclusion Phases of Arbitrary Ellipsoidal Shape. *Journal of Engineering Mechanics*, Vol. **136**, pp. 1043-1053, 2010.

[12] J.C. Simo and T.J.R Hughes. Computational Inelasticity. *Springer: Interdisciplinary Applied Mathematics*, Vol. **7**, 1998.