Multi-scale modeling of polysaccharide and protein based aerogels

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Polysaccharide and protein based aerogels are a class of highly porous organic aerogels, widely used in the biomedical industry. These aerogels are characterized by a cellular morphology and their macroscopic mechanical behavior is based on the mechanics of their cell wall fibrils. In our study, two models are presented. The compression model is based on the bending and compression of the cell wall fibrils [1]. Large deformations are accounted for by using the extended Euler-Bernoulli beam theory [2]. On the other hand, the tension model is based on the bending and stretching of the cell wall fibrils [3]. Under tension, aerogels only undergo small deformations. Accordingly, their behavior is captured using the standard Euler Bernoulli beam theory. The damage and failure mechanisms are based on the critical stresses generated in the cell wall fibrils. The network of microcells is defined using the pore size distribution data obtained via the Barrett-Joyner-Halenda (BJH) model. The model predictions are validated against experimental data.

This microcell based modeling idea is also extended to capture the effect of wetting on their mechanical response. Due to wetting, the water-filled pores provide impedance to the bending deformation of the cell walls. This resistance to deformation is modeled by Winkler-type of elastic foundation for the cell walls. The so resulting stiffness of the foundation is then correlated to the water content. A constitutive model is thus proposed, and its results are validated against experimental data.

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[2] Jenkins J.A., Seitz T.B., and Premieniecki J.S. (1966) Large deflections of diamond-shaped frames. Int. J. Solids Struct. 2, 591-603.

[3] Rege A. and Itskov M. (2017) A microcell based constitutive modeling of cellulose aerogels under tension. Acta Mech. (in press)