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CELL WALL PROPERTIES OF NANOFIBRILLAR CELLULOSE FOAMS FROM TOMOGRAPHY AND SIMULATIONS

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Summary: X-ray tomography scans of NFC foams are used to reconstruct structures, which are then discretised and used in finite element simulations. Structures which are obtained by thresholding the scans at different levels are used in these simulations to obtain the constants that govern the material scaling laws. These constants in conjunction with experimental results are then used to determine constitutive solid material properties of NFC foam cell walls.

1. INTRODUCTION

Nanofibrillar cellulose (NFC) based materials, owing to their interesting mechanical, thermal, acoustic and chemical properties, have elicited considerable interest in the recent past. An interesting material derived from NFC as the building block is the NFC foam. It is a porous material exhibiting cellular microstructure and has been proposed for applications in industries ranging from the automotive to the biochemical. In applications where the mechanical properties of these foams are of importance, it is necessary to develop reliable finite element models so that the behaviour of these foams in structural applications can be studied in detail. In such simulations, the constitutive properties of the material that make up these foams (referred to here as the cell wall properties) are of importance. The experimental methods to determine these properties are limited by the length scales involved, as it is difficult to perform the traditional mechanical tests by isolating the material in the cell walls. Indirect methods, like indentation testing on NFC thin films, are usually not representative of the cell wall material. Our work addresses this issue by combining x-ray tomography and finite element simulations to determine the cell wall properties.

2. TOMOGRAPHY SCANS AND SIMULATIONS

The tomography scans in this study were obtained from the 4D-Imaging lab, Division of Solid Mechanics, Lund University. Cylindrical NFC foam samples of size 600 microns in diameter and 600 microns in height were scanned with a voxel size of 600 nm. The image processing software Avizo® was used to process the scans and extract the surface of the NFC foams. This was accomplished by a series of image processing operations comprising of histogram equalisation, thresholding and island removal. The structure that is so obtained is not always continuous and has disconnected strands of material. As the finite element analysis necessitates a continuous structure, the structure is further processed in Matlab® to obtain a single continuous structure. This geometry is then discretised (see Fig. 1(a)) in the finite element meshing software Hypermesh®, before being subject to large strain compressive loading.

The process of thresholding the scans introduces uncertainty into the determination of structure and voids. Objectively, after thresholding the ratio of structure to void volume must correspond to the known global porosity of the foams scanned. However, given the size of the sample that is scanned, it is seen that trying to attain the global porosity level results in loss of structural detail. Also, it is not necessary that the local porosity (of the small sample that is scanned) be equal to the global porosity of the foam. Thus, we obtain structures of increasing porosity by thresholding them progressively. The material property scaling laws relate the constitutive solid and bulk properties to the relative density (porosity) of the material [1]. The constants in these relations are related to the geometry of the structure and the nature of deformation (see equation 1). We determine these constants from the simulation of

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reconstructed structures of different porosities. These are then used in conjunction with experimental results to obtain the constitutive solid material properties of NFC foams (see equation 2) [2].

$$\frac{E^*}{E_s} = C_1\left(\frac{\rho^*}{\rho_s}\right)^{n_1} \text{ and } \frac{\sigma_p}{\sigma_{ys}} = C_2\left(\frac{\rho^*}{\rho_s}\right)^{n_2}\text{; '}*\text{' and 's' refers to the bulk and constitutive solid properties respectively} \quad (1)$$

$$E_s = \frac{E^*_{exp}}{\overline{C_1}\left(\frac{\rho^*}{\rho_s}\right)^{\overline{n_1}}} \text{ and } \sigma_{ys} = \frac{\sigma_{ys,exp}}{\overline{C_2}\left(\frac{\rho^*}{\rho_s}\right)^{\overline{n_2}}} \text{ ; } \overline{C_1}, \overline{C_2}, \overline{n_1} \text{ and } \overline{n_2} \text{ are averaged constants obtained from simulation} \quad (2)$$

3. RESULTS

We estimate the elastic modulus and the yield strength of the cell walls in NFC foams to be 29.78 GPa and 40.76 MPa respectively. The estimate of the elastic modulus is high compared to the earlier estimates by indirect methods (8.65 GPa by Ali et al. [3] and 3.9 – 5.7 GPa. Gordeyeva et al. [4]) but compares favourably to the highest estimate for cellulose nanopaper. The finite element simulations also corroborate the nature of deformation, i.e. through hinge formation followed by plastic collapse, as observed in the in-situ measurements by Martoïa et al. [5]. The simulations also provide a validation case for numerical reconstruction of the geometry of NFC foams and their simulation.

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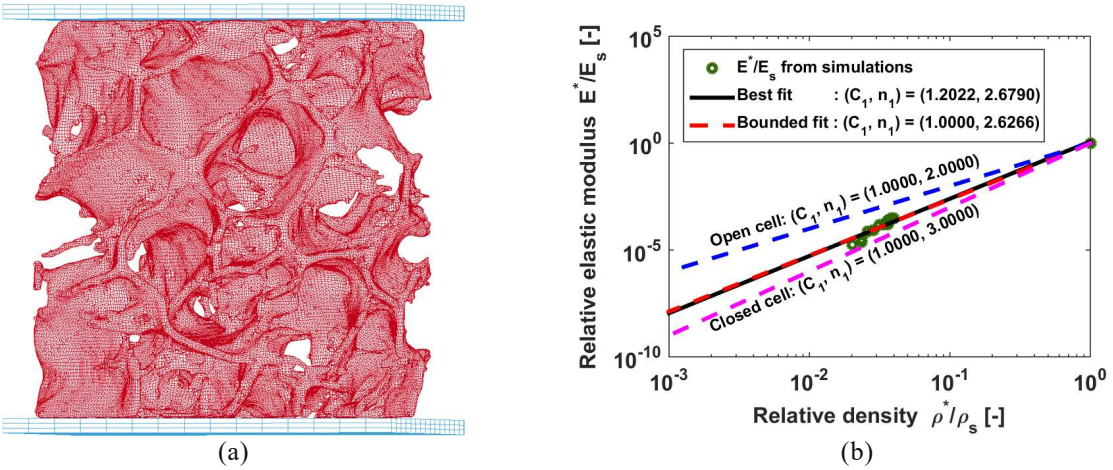

(a) (b)

Figure 1: (a) An example of the discretized foam structure that is reconstructed from the tomography scan. (b) The results from fitting the simulation data to the elastic material property scaling laws [2].