6th European Conference on Computational Mechanics (ECCM 6)
7th European Conference on Computational Fluid Dynamics (ECFD 7)
11 – 15 June 2018, Glasgow, UK

MULTISCALE MODELING OF CRYSTALLINE CELLULOSE MICROFIBRIL INTERFACE

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Key Words: *crystalline cellulose, interface, moisture, hygro-mechanical behavior, molecular dynamic, finite element*

Plants and natural materials such as wood, in wet state, may undergo large deformation without failure. Inspired by microscopic observation of the existence of contacts in microfibrils networks within the plant cell wall (Cosgrove 2014), we investigate computationally, using a multiscale modeling framework, how crystalline cellulose microfibrils in contact with each other may play an important role in the hygro-mechanical behavior of plant.

Cellulose is the most abundant biopolymer on earth. Cellulose consists in chains of glucose monomer assembled in the Iβ crystalline form in softwood. Microfibrils, consisting of chains of cellulose crystals, are the major load bearing components of plant cell wall. Looking at one crystal, we focus on two different planes of microfibril (Figure 1), *i.e.* one is hydrophilic (110) and the other hydrophobic (200) and study different contacts configuration, in presence or absence of water. 48 different configurations with varying moisture amount and angle between crystal main axes and contact plane, are investigated by Molecular Dynamics (MD) to capture to fine level contact behaviour. The results show that the microfibril with square cross-section is less stable than the hexagonal one, as single or double chains lying on plane (200) are likely disrupted. Contacts between two hydrophilic (110) planes show a stick-slip behavior under shear loading. Finally, we found that interfacial moisture significantly reduces the sliding and bonding strength, yet normal stresses, both compressional and tensile, do not affect strongly the bonding and sliding strength (Figure 2).

The constitutive behaviour of the contact is derived from these MD simulations, and then implemented in a finite element model using contact elements for investigating the interfacial behavior at larger scale. First, we control that consistency between MD and FEM is achieved. Then, modeling with FEM a larger material area in the S2 layer of wood loaded under common stress levels experienced by wood in use, we found that moisture is an activator for loosening the bonding at microfibril interface, yielding large deformations due to interface sliding not possible under dry condition.

In this study, we investigate the mechanical behavior of the microfibril interface, especially the influence of interfacial moisture, using a multiscale modeling framework, taking the advantage of both continuum and atomistic simulation approaches.

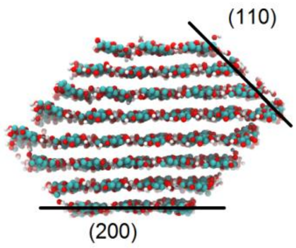

Figure 1 hexagonal cross-section of microfibril, the two types of surfaces hydrophilic (110) and hydrophobic (200) are indicated

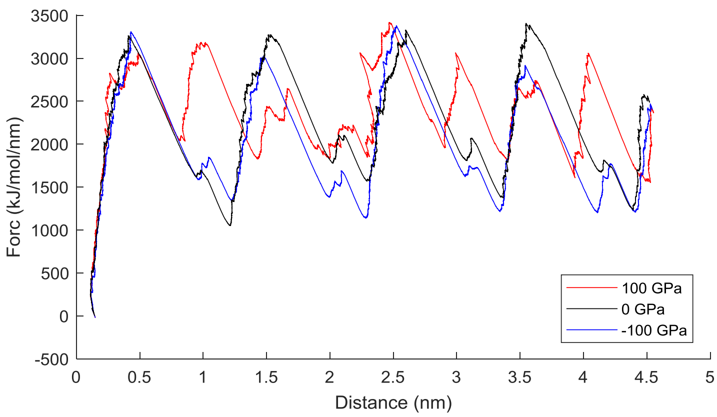

Figure 2 influence of compressional and tensile stresses on stick-slip behavior of dry interface between (110) and (110) plane, with main axes aligned, showing similar peak forces of the three conditions.

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