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Research Paper

Molecular deformation mechanisms of the wood cell wall material

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ABSTRACT

Wood is a biological material with outstanding mechanical properties resulting from its hierarchical structure across different scales. Although earlier work has shown that the cellular structure of wood is a key factor that renders it excellent mechanical properties at light weight, the mechanical properties of the wood cell wall material itself still needs to be understood comprehensively. The wood cell wall material features a fiber reinforced composite structure, where cellulose fibrils act as stiff fibers, and hemicellulose and lignin molecules act as soft matrix. The angle between the fiber direction and the loading direction has been found to be the key factor controlling the mechanical properties. However, how the interactions between theses constitutive molecules contribute to the overall properties is still unclear, although the shearing between fibers has been proposed as a primary deformation mechanism. Here we report a molecular model of the wood cell wall material with atomistic resolution, used to assess the mechanical behavior under shear loading in order to understand the deformation mechanisms at the molecular level. The model includes an explicit description of cellulose crystals, hemicellulose, as well as lignin molecules arranged in a layered nanocomposite. The results obtained using this model show that the wood cell wall material under shear loading deforms in an elastic and then plastic manner. The plastic regime can be divided into two parts according to the different deformation mechanisms: yielding of the matrix and sliding of matrix along the cellulose surface. Our molecular dynamics study provides insights of the mechanical behavior of wood cell wall material at the molecular level, and paves a way for the multi-scale understanding of the mechanical properties of wood.

Introduction

Wood, with its broad availability, has served as an important bulk material since ancient times and still plays a major role today. One important application area of wood is in the load bearing systems, for example, houses, bridges, ships and even aircrafts, since it also possesses excellent mechanical properties. In the sense of specific mechanical properties (normalized by mass density), wood material parallels and even behaves better than many other engineering materials

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such as steel (Ashby et al., 1995; Gibson and Ashby, 1999; Gibson et al., 1995). In fact, the origin of most woods, the tree, is also a load bearing system, where the smart design of the wood structure renders a tree capable of supporting its own weight and sustaining various climate conditions (Fratzl and Weinkamer, 2007; Qin et al., 2014). The unique combination of composite material and microstructure design in wood material has attracted research interests in comprehensive understanding the mechanical properties of wood and designing inspired materials and structures (Compton and Lewis, 2014; Gibson and Ashby, 1999; Gibson et al., 2010).

Similar to other outstanding biological materials, for example, spider silk (Eisoldt et al., 2011; Keten et al., 2010), bone (Launey et al., 2010; Nair et al., 2013; Weiner and Wagner, 1998) and sponge (Aizenberg et al., 2005; Meyers et al., 2013), wood also features a hierarchical structure (Ali and Gibson, 2013) (Fig. 1). At the macro-scale, we can clearly see the annual rings in a cross-section of a wood trunk (Fig. 1**a**), which is a result of the different growing rates during different seasons (Fratzl and Weinkamer, 2007). Zooming into the micrometer scale, we can clearly see that the wood material is not solid but features a cellular structure (Fig. 1**b, c**), where hollow space is enclosed by wood cell walls. Studies have shown that the cellular structure is the underlying feature that endows wood as an excellent mechanical material: it makes wood light weight and perform efficiently when it is used as engineering components (Ashby et al., 1995; Gibson and Ashby, 1999; Gibson et al., 1995; Vural and Ravichandran, 2003). The significant hollow space in wood also gives it high deformability. For example, cork is an excellent material for energy absorption and bottle bungs (Gibson and Ashby, 1999).

As shown in Fig. 1**c-e**, the wood cell wall material is a composite, combing stiff and soft polymer components. Studies have shown that the wood cell wall is composed of multiple layers and it is a kind of fiber-reinforced composite with stiff cellulose fibrils embedded in soft matrix consisting of hemicellulose and lignin (Booker and Sell, 1998; Fahlen and Salmen, 2002) (Fig. 1**c, d**). Among these layers, the middle layer of the secondary cell wall (S2 layer), which occupies more than 80% of the thickness of the cell wall, is the thickest and mainly controls the mechanical properties of the wood cell wall (Booker and Sell, 1998). A unique feature of S2 layer is that the stiff cellulose fibrils lie parallel with each other and form an angle (micro-fibril angle, MFA) with the longitudinal axis of wood cell (Fig. 1**d**) (Booker and Sell, 1998). As the longitudinal direction is the main load-bearing direction in wood, the mechanical properties of wood mainly relate to the cell wall's properties along this direction. Since MFA measures how close are the stiff cellulose fibrils aligned with this load-bearing direction, it plays a key role in controlling the mechanical properties of wood cell wall: smaller MFA indicates that the stiff cellulose fibrils are more aligned with the load-bearing direction, and the material will behave stiffer. (Booker and Sell, 1998; Navi et al., 1995; Reiterer et al., 2001; Reiterer et al., 1999). Since the stiff cellulose fibrils spirally wind the wood cell (Booker and Sell, 1998), tensile loading along the longitudinal direction will result in the unwinding of the fibrils and the decreasing of the MFA (Keckes et al., 2003). Theoretical and simulation works have proposed that this reorientation of the fibrils generates relative shearing between adjacent fibrils, and that the shear deformation on the matrix is the underlying mechanical response that is responsible for the mechanical

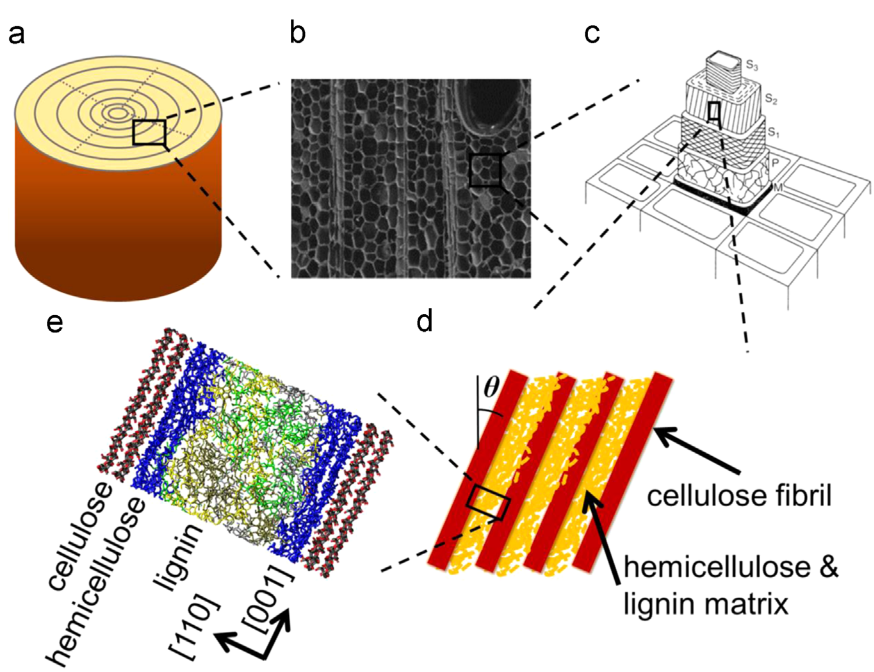

Fig. 1 – The hierarchical structure of wood material. (a) A drawing shows the annual rings structure at the cross-section of a wood trunk. (b) The cellular structure of wood (reproduced from (Vural and Ravichandran, 2003), with permission from Elsevier). (c) Multiple layers in wood cell wall (reproduced from (Booker and Sell, 1998), with permission from Springer). M: middle layer, P: primary layer, S1: the first secondary layer, S2: the second secondary layer, S3: the third secondary layer. (d) The fiber reinforced structure of wood cell wall. The stiff fibrils form an angle θ (micro-fibril angle, MFA) with the longitudinal direction of cell. (e) The molecular model used in the present study. Black arrows indicate the crystal orientations of cellulose.