Crystalline Cellulose – Atomistic Modeling Toolkit

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Nature has created efficient strategies to make materials with hierarchical internal structure that often exhibit exceptional mechanical properties. One such example is found in cellulose, in fact it is eight times stronger than stainless steel and advantage is that cellulose incredibly cheap, because processing is obtained from purified wood pulp (it is environmental friendly). The most prevalent modeling technique to study the fundamental mechanical behavior of the crystalline cellulose has been Molecular Dynamics (MD). As a predictive tool, MD allows us to study the behavior of crystalline cellulose at the atomic level, and as such, it accurately predicts the crystalline structure, covalent bonds and non-bonded interactions. State-of-the-art in-situ electron microscopy and atomic force microscopy experimental techniques can provide rich information about the structure and mechanics of these materials as well. However, interpretation of this experimental data requires the combination with modeling. Current efforts are focused on the development of an atomistic simulation toolkit that will allow us to run MD simulations to study the nonlinear structural behavior of cellulose chains and their interactions in crystalline cellulose.