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Cellulose microfibril formation within a coarse grained molecular dynamics[1] ABDOLMADJID NILI, OLEG SHKLYAEV, VINCENT CRESPI, ZHEN ZHAO, LINGHAO ZHONG, The Pennsylvania State University, CLSF COLLABORATION — Cellulose in biomass is mostly in the form of crystalline microfibrils composed of 18 to 36 parallel chains of polymerized glucose monomers. A single chain is produced by cellular machinery (CesA) located on the preliminary cell wall membrane. Information about the nucleation stage can address important questions about intermediate region between cell wall and the fully formed crystalline microfibrils. Very little is known about the transition from isolated chains to protofibrils up to a full microfibril, in contrast to a large body of studies on both CesA and the final crystalline microfibril. In addition to major experimental challenges in studying this transient regime, the length and time scales of microfibril nucleation are inaccessible to atomistic molecular dynamics. We have developed a novel coarse grained model for cellulose microfibrils which accounts for anisotropic interchain interactions. The model allows us to study nucleation, kinetics, and growth of cellulose chains/protofibrils/microfibrils.

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