Abstract Submitted
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Effect of Intrinsic Twist on Length of Crystalline and Disordered Regions in Cellulose Microfibrils[1] ABDOLMADJID NILI, OLEG SHKLYAEV, ZHEN ZHAO, LINGHAO ZHONG, VINCENT CRESPI, Pennsylvania State University — Cellulose is the most abundant biological material in the world. It provides mechanical reinforcement for plant cell wall, and could potentially serve as renewable energy source for biofuel. Native cellulose forms a non-centrosymmetric chiral crystal due to lack of roto-inversion symmetry of constituent glucose chains. Chirality of cellulose crystal could result in an overall twist. Competition between unwinding torsional/extensional and twisting energy terms leads to twist induced frustration along fibril's axis. The accumulated frustration could be the origin of periodic disordered regions observed in cellulose microfibrils. These regions could play significant role in properties of cellulose bundles and ribbons as well as biological implications on plant cell walls. We propose a mechanical model based on Frenkel-Kontorova mechanism to investigate effects of radius dependent twist on crystalline size in cellulose microfibrils. Parameters of the model are adjusted according to all-atom molecular simulations.

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