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Coarse-Grained Simulation of Solvated Cellulose Ib Microfibril BINGXIN FAN, Department of Chemical Engineering, Penn State University, JANNA MARANAS, Department of Chemical Engineering and Material Science, Penn State University, DR. LINGHAO ZHONG AND DR. ZHEN ZHAO COLLABORATION — We construct a coarse-grained (CG) model of cellulose microfibrils in water. The force field is derived from atomistic simulation of a 40 glucose-unit-long microfibril by requiring consistency between the chain configuration, intermolecular packing and hydrogen bonding of the two levels of modeling. Intermolecular interactions such as hydrogen bonding are added sequentially until the force field holds the microfibril crystal structure. This stepwise process enables us to evaluate the importance of each potential and provides insight to ordered and disordered regions. We simulate cellulose microfibrils with 100 to 400 residues, comparable to the smallest observed microfibrils. Microfibrils longer than 100nm would form a bending region along their longitudinal direction. Multiple bends are observed in the microfibril containing 400 residues. Although the cause is not clear, the bending regions may provide us insights about the periodicity and the behavior of the disordered regions in the microfibril.

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