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Nanomechanics of Incipient Kink Defects Formed in Nanocellulose

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ABSTRACT

Kink defects in nanocellulose are ubiquitous yet associated questions remain open regarding the unclear microstructure-mechanical property relationship. Various kink patterns without molecular-scale resolution result in bemusements of how nanocellulose forms different kinks and what the fundamental mechanisms of reversible and irreversible kinks are. In our atomic force microscopy images of mechanically treated cellulose nanofibrils, bent nanofibrils usually exhibit small curvatures while kinked nanofibrils feature sharp bends, in which kinks are conspicuous due to their promiscuous configurations. To identify the nanomechanics of incipient kink defects formed in nanocellulose, molecular dynamics simulations of cellulose nanocrystals (CNCs) under curvature-dependent bending are subsequently carried out. Four typical bending/kinking modes are found, depending on the anisotropic microstructure and size of CNCs. More importantly, two contrasting cases of kinks are demonstrated, providing evidence that kink defects in nanocellulose depend mainly on the microstructure at the molecular scale. Kinks in CNCs with the van der Waals interface are recoverable with a few residual defects. While kinks in CNCs with the hydrogen-bonding interface are irreversible with permanent microstructural damage due to the less ordered molecular chains and destroyed hydrogen-bonding network. Compressive stresses accumulated in the bottom chains of CNC contribute to the main mechanism to form incipient kinks in nanocellulose. Layer number is found to be the main size parameter dominating the bending/kinking of CNCs. Our experiments and simulations present intrinsic deformation mechanisms for reacquainting ubiquitous but mysterious kinks arising in nanocellulose, in which the distinctive insights should provide guidelines for cellulose-based biomass conversion and hierarchical material design with tailored properties.

KEYWORDS

Nanocellulose; kink deformation; kink defects; bending; hydrogen bond

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