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PROCEEDINGS

Intrinsic Deformation Mechanism of Nanocellulose

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ABSTRACT

Kink defects are prevalent in nanocellulose. The existence of diverse kink patterns lacking molecular-scale resolution has caused uncertainty regarding the mechanisms governing the formation of different kinks in nanocellulose, including both reversible and irreversible kinks. The constraints resulting from these limitations often lead to significant confusion in exploring the structure-property relationships of nanocellulose. By integrating AFM experiments with molecular dynamics simulations, we examined the microstructure-dependent kink deformations in nanocellulose (Iβ phase) and the resultant local microstructural damages. In atomic force microscopy images, bent nanofibrils typically display minor curvatures, whereas kinked nanofibrils exhibit pronounced sharp bends, wherein the kinks are conspicuous owing to their discernible disordered configurations. To identify the incipient kink defects formed in nanocellulose, molecular dynamics simulations of cellulose nanocrystals (CNCs) were subsequently conducted. The curvature-controlled bending method was employed to investigate the bending and kinking responses of CNCs along different crystal planes. Five typical bending/kinking modes were discovered, and two contrasting cases of kinks were demonstrated, providing evidence that kink defects in nanocellulose primarily depend on the microstructure at the molecular scale. Compressive stresses accumulated in the bottom chains of CNCs contribute to the main mechanism for forming incipient kinks in nanocellulose. These insights offer intrinsic deformation mechanisms for comprehending the widespread yet enigmatic kinks observed in nanocellulose.

KEYWORDS

Nanocellulose; molecular disorganization; kink defects; hydrogen bond

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