

Experimental and Modeling Investigation of Cellulose Nanocrystals Polymer Composite Fibers

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Abstract:

Cellulose nanocrystals (CNCs) are a class of newly developed and sustainable nanomaterial derived from cellulose-based materials such as wood. There have been substantial research efforts to utilize these materials as reinforcing agents. However, in order to develop CNC nanocomposites with industrial applications, it is necessary to understand how addition of CNCs affect the properties of the polymer nanocomposite. In the present work, several approaches, experimental and theoretical, are presented in an effort to characterize and understand the effect of CNCs on the properties of polymer CNC fibers.

Two experimental methods were used to develop cellulose acetate (CA) and CNC composite fibers: electrospinning and dry spinning. Polyvinyl alcohol (PVA) and CNC dry spun composite fibers were also produced in order to study the effect of CNCs in additional polymeric systems. Surface morphology of these fibers was analyzed by scanning electron microscopy and optical microscopy. Elastic modulus, elongation, and ultimate tensile strength were measured by dynamic mechanical analysis. CNC dispersion was assessed by optical microscopy under cross polarizers. 2D X-ray diffraction was used along with the Herman's order parameter to quantify the level of orientation of the CNCs within the dry spun fibers.

It was found that the orientation of the CNCs within the fiber directly correlates to the mechanical properties of the composite. Continual improvement in the tensile

strength and elastic modulus of the fibers were observed until a critical concentration. Further increases in CNC concentration did not yield corresponding improvement and led to large variations in fiber performance, likely due to increased defect density and/or aggregation of CNCs. Empirical micromechanical models Halpin-Tsai equation and an orientation modified Cox model were used to predict the fiber performance and compared with experimental results.

Finally, a one dimensional model is presented using fundamental equations of momentum, mass and energy, along with a modified Pipes viscous constitutive equation to predict the diameter, velocity, component concentration, and temperature profile of the dry spinning system. Sensitivity analysis was performed on various spinning parameters such as mass flow rate, temperature of the spinning dope and air, the velocity of take-up speed, and the velocity of the quenched air. In addition, the effect of CNCs' orientation on the system was also investigated. It is found that perfectly collimated CNCs increased the elongational viscosity of the system, thus resulting in a thicker fiber.

The methods and results presented in this work help describe the behavior of polymer-CNC composites and may serve as a useful tool for process optimization of such materials. Based on these results, this study shows that for near collimated states of orientation, the CNCs provide an excellent form of polymer reinforcement and may contribute to the field as a renewable, lightweight and strong nanomaterial.