ELECTROSPINNING OF CELLULOSE NANOCRYSTALS

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Electrospinning cellulose nanoparticles in cellulose acetate solutions using Acetone/Acetic acid as solvents offers a promising approach for producing high-performance cellulose fibers that can reinforce composites with exceptional mechanical properties. However, electrospinning cellulose alone is a challenging process. Therefore, cellulose acetate fibers are electrospun first, then deacetylated and regenerated back to cellulose. The alignment of cellulose nanocrystals along the electrospun fibers is crucial in providing the desired mechanical properties to the composite material. In this study, we use KOH to regenerate cellulose fibers (Fig 1(R)) and further utilize molecular dynamics simulations to investigate the effects of various factors such as the cellulose acetate polymeric chains, filler type (i.e., cellulose nanocrystals or nanofibrils), and the overall composition on the electrospinning process and filler alignment.

Our results suggest that the cellulose acetate polymeric chains align well on the surface of the fillers and form connections between them, leading to the alignment of the filler particles along the electrospun fibers. Furthermore, we observed that the alignment of the cellulose acetate polymers themselves is also affected by the concentration of the constituents and the type of filler. However, we also found that the use of Acetone/Acetic acid significantly decreased the dynamics of the system compared to water solutions. The movement of the fillers in Acetone/Acetic acid solutions was comparably slower than in water solutions. Despite the higher dynamics of water, it cannot be used to electrospin cellulose in practice. Our ongoing simulations and experiments aim to further elucidate the underlying mechanisms governing the electrospinning process and the effects of different solvent systems on the filler alignment and mechanical properties of the composite material.

In addition, our upcoming research will focus on exploring the in-situ regeneration of cellulose from cellulose acetate solutions, in contrast to the current multi-step deacetylation process. This step is crucial and innovative in the electrospinning process suggested by our study, for obtaining fibres with exceptional mechanical performance. Regeneration affects the properties of the electrospun fibers, such as their porosity and mechanical strength, and understanding the underlying mechanisms can aid in the design of high-performance sustainable composite materials.

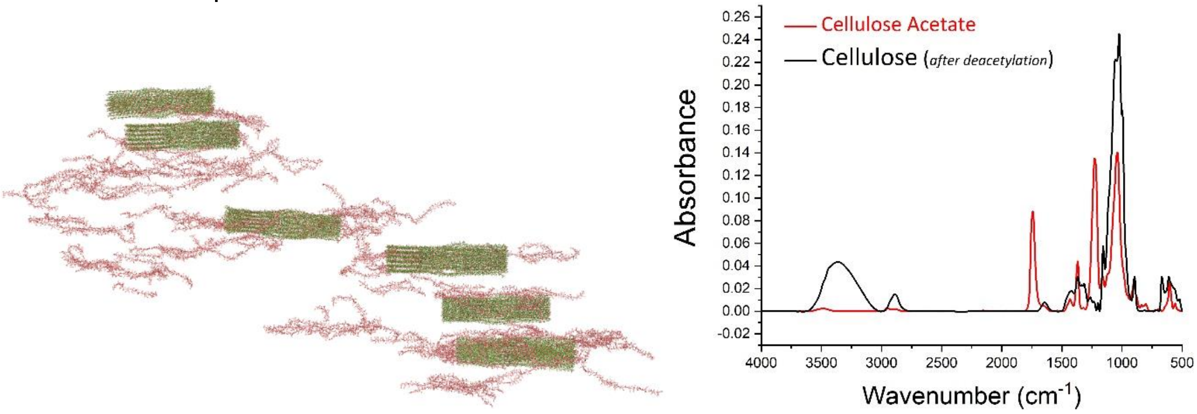

Figure 1: (L) A snapshot of the cellulose nanofibrils in a solution of cellulose acetate, aligned by the electric field. (R) FT-IR Spectra peaks confirming regenerated cellulose.