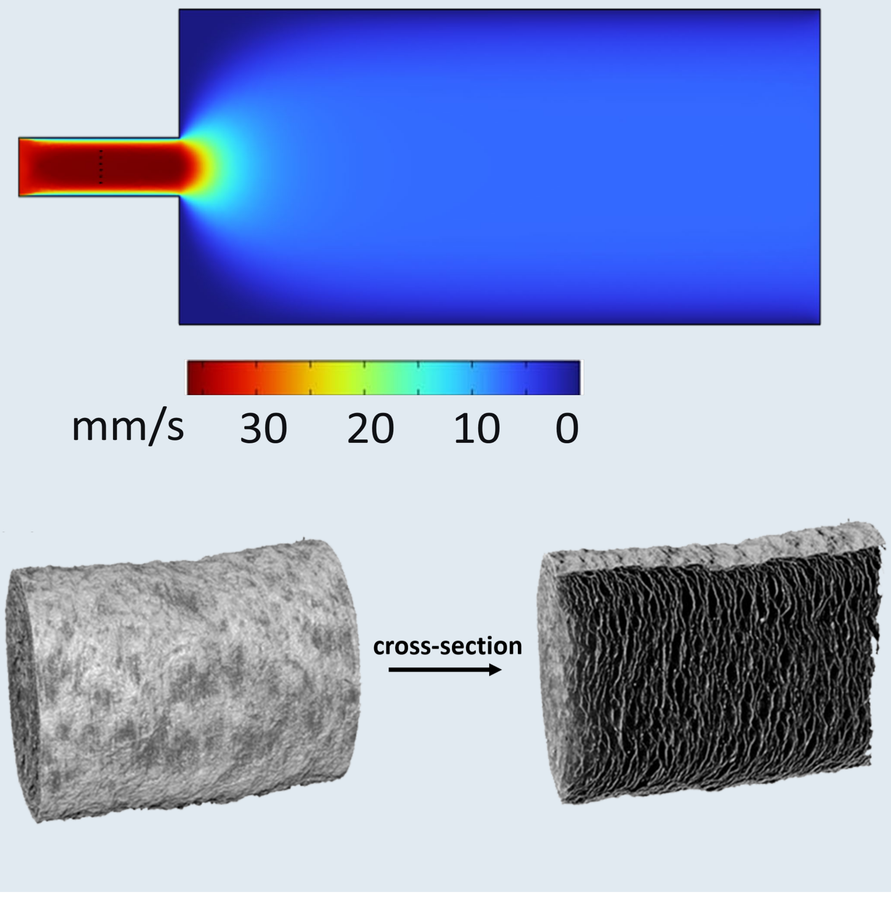


Flow-Regime-Controlled Fabrication of Vertically-Aligned 2D-Nanosheet Fibers

This research reveals that expansion flow generates nanosheet alignment, whereas subsequent plug flow suppresses shear-induced reorientation and preserves the vertically aligned structure.

Tuxiang Guan, Yue Han, Mengjie Li

State Key Laboratory of Materials-Oriented Chemical Engineering, Nanjing Tech University

Abstract

COMSOL Multiphysics was employed to investigate the flow behavior of non-Newtonian graphene oxide (GO) dispersions in an expansion spinneret. By coupling experimentally measured rheological properties with computational fluid dynamics, the evolution of velocity and shear-rate fields was analyzed under different crosslinker concentrations. The simulations reveal a sequential expansion-flow-to-plug-flow transition at high viscosity: expansion flow drives nanosheet rotation, while the low-shear plug-flow region preserves the generated vertical alignment. In contrast, low-viscosity dispersions develop laminar flow with pronounced velocity gradients, resulting in shear-induced structural disruption.

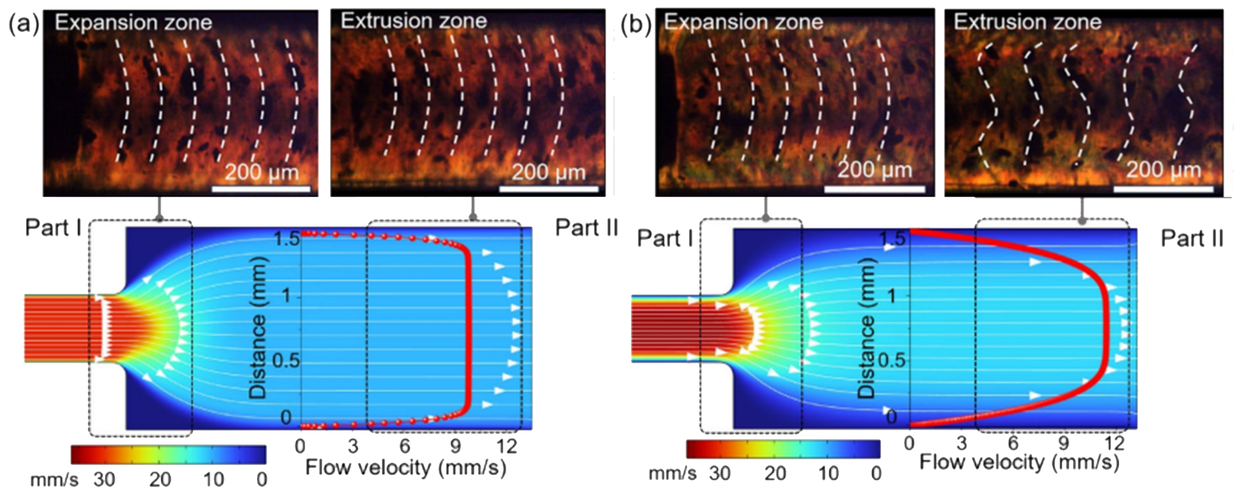


Figure 1. Flow field variation of GO dispersion with crosslinker ratio of a) 30%, and b) 0%.

Methodology

The flow dynamics of 2D material dispersions in an expansion channel were investigated using the Laminar Flow module in COMSOL Multiphysics. The rheological properties of the dispersion employed in the simulation were determined by fitting the viscosity-shear rate curve. The geometric model was discretized using a free triangular mesh, with additional boundary layer meshing applied to boundary layer regions. The governing fluid dynamics equation is expressed as: $\rho(u\cdot\nabla)u = \nabla\cdot[-pI+K]+F$.

Results

- At 0% crosslinker, nanosheets temporarily flip vertical in expansion zone. Subsequent laminar-flow generates parabolic velocity profile and widespread high-shear regions. Violent angle fluctuation disrupts pre-established vertical microstructure.
- At 30% crosslinker, expansion-zone extensional stress orients nanosheets vertically. Downstream plug-flow delivers uniform cross-section velocity and low shear rate. Nanosheet deflection angles remain stable, vertical alignment is well preserved.

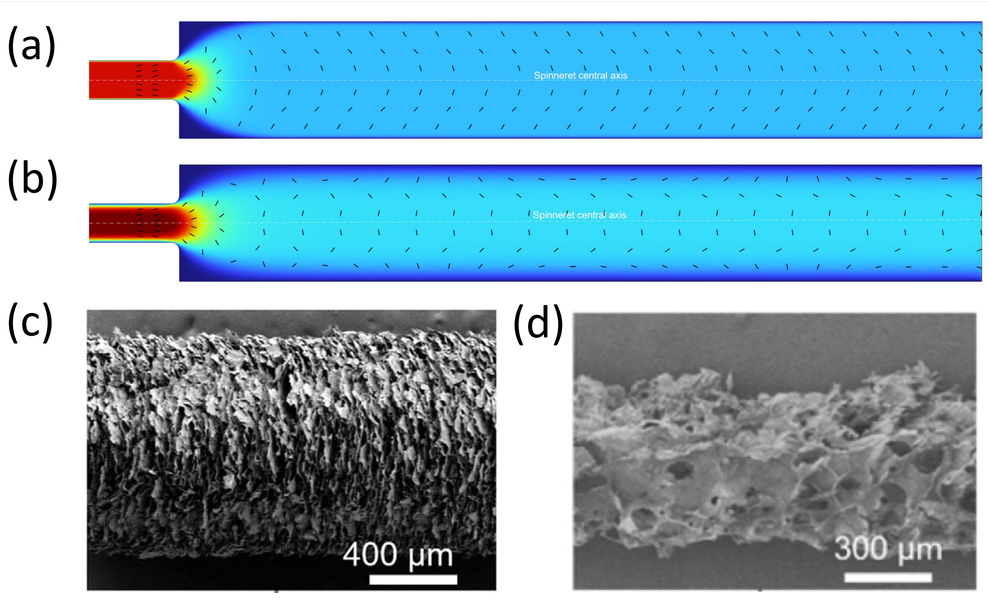


Figure 2. Summary of simulation results for GO nanosheets deflection trajectory, with crosslinker ratio of (a) 30%, and (b) 0%;SEM images of fibers of (c) 30% and (d) 0%.

References

Guan T, Hu W, Shen S, et al. Flow-Regime-Controlled Fabrication of CNT-Bridged Vertically Aligned rGO/MXene Fibers for High-Performance Fiber Supercapacitors[J]. *Advanced Materials*, 2025, e202516561.

NANJING TECH UNIVERSITY

南京工業大學

Excerpt from the Proceedings of the COMSOL Conference 2026 Shenzhen