Molecular Dynamics Simulations of Polymeric Fibre Bundles under Tensile Load

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Bundles of polymeric materials play essential and ubiquitous roles in biological systems, and often display remarkable mechanical properties [1]. By preforming non-equilibrium molecular dynamics simulations of polymeric fibre bundles under tensile load one gets valuable insight into the mechanical properties of nanofibrous materials. This allows for investigation of the role of the supra-molecular structure of fibrils in nanometric bundles of polymeric material, which have been shown experimentally to have a great impact on e.g. the Young's modulus of the bundles [2]. As bio-fibres do not exist or operate in vacuum, we also consider the effects of adding third species, such as room temperature ionic liquids (RTIL's) and aqueous environments. RTIL's constitute a vast class of systems, displaying an equally huge variety of properties [3]. Some have shown promising results as a solvent for cellulose, which is relatively insoluble in water due to its large number of intra-molecular hydrogen bonds [4][5], and little is known about how this dissolution would affect the mechanical properties. Further, we aim to explore the fibril-equation of state and create a connection between the behavior of nanometric polymers under tensile load to the Fibre Bundle Model [6], which for over a century has been the leading theoretical framework to investigate fracture in fibrous materials on the macroscopic scale.

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