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Dynamics and topology of a flexible chain: knots in steady shear flow AGNIESZKA SLOWICKA, Institute of Fundamental Technological Research, Polish Academy of Sciences, Pawinskiego 5b, 02-106 Warsaw, Poland, STEVE KUEI, Rice University, Department of Chemical and Biomolecular Engineering, Houston, TX 77005, USA, MARIA EKIEL-JEZEWSKA, ELIGIUSZ WAJNRYB, Institute of Fundamental Technological Research, Polish Academy of Sciences, Pawinskiego 5b, 02-106 Warsaw, Poland, HOWARD STONE, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton NJ 08544, USA — Dynamics of particles in a water-base liquid is a very important subject of research from the point of view of biological, medical and industrial applications. Motion of microorganisms, biopolymers, proteins or artificial particles immersed in a flowing liquid is complex and such systems have numerous applications but, on the other hand, the dynamics has not been yet very well understood. I our paper we performed numerical simulations of a bead-spring model chain to investigate the dynamics of long and flexible elastic fibers in a steady shear flow. For a class of rather open conformations and different parameters of flexibility, we identify two district conformational modes with different final size, shape, and orientation. Through further analysis we identify slipknots in the chain. We also analyzed evolution of the fibers which initially form "open" trefoils for different chain flexibilities and initial orientations with respect to the flow direction. We found examples, which illustrate that the shear flow can unknot a flexible chain and then knot it again; this phenomenon sometimes repeats several times.

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