

Abstract Submitted
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Threading events in ring polymer melts: a detailed geometric analysis and their connection with the slow relaxation modes VLASIS MAVRANTZAS, DIMITRIOS TSALIKIS, University of Patras, DIMITRIS VLASSOPOULOS, University of Crete FORTH-IESL — We will present results from a detailed geometric analysis of atomistic configurations of ring polyethylene oxide melts accumulated in the course of very long molecular dynamics (MD) simulations at $T = 413\text{K}$ and $P = 1\text{atm}$ which allowed us to locate ring-ring threading events and quantify their strengths and survival times. We have identified a variety of threading situations and studied their dependence on ring molecular weight. We have found that threadings can last up to several times the corresponding ring relaxation time, which can explain (at least in part) the appearance of slow relaxation modes observed experimentally in entangled polymer rings [2]. We confirm this by proposing a new expression for the stress relaxation modulus of entangled polymer rings that is found to provide excellent fits to experimentally measured curves. [1] D.G. Tsalikis, V.G. Mavrantzas, D. Vlassopoulos, *ACS Macro Lett.* 5, 755 (2016). [2] M. Kapnistos, M. Lang, D. Vlassopoulos, W. Pyckhout-Hintzen, D. Richter, D. Cho, T. Chang, M. Rubinstein, *Nature Materials* 7, 997 (2008).

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