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New Insight in Understanding the mechanical responses of polymer glasses using molecular dynamic simulation[1] YEXIN ZHENG, SHIQING WANG, MESFIN TSIGE, Department of Polymer Science, University of Akron — The Kremer-Grest bead-spring model has been the standard model in molecular dynamics simulation of polymer glasses. However, due to current computational limitations in accessing relevant time scales in polymer glasses in a reasonable amount of CPU time, simulation of mechanical response of polymer glasses in molecular dynamic simulations requires a much higher quenching rate and deformation rate than used in experiments. Despite several orders of magnitude difference in time scale between simulation and experiment, previous studies have shown that simulations can produce meaningful results that can be directly compared with experimental results. In this work we show that by tuning the quenching rate and deformation rate relative to the segmental relaxation times, a reasonable mechanical response shows up in the glassy state. Specifically, we show a younger glass prepared with a faster quenching rate shows glassy responses only when the imposed deformation rate is proportionally higher.

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