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Molecular dynamics study of reversible thermal stiffening in viscoelastic polymer blends and nanocomposites WEI PENG, RAGHAVAN RANGANATHAN, FIONA KINE, RAHMI OZISIK, PAWEL KEBLINSKI, Rensselaer Polytech Inst, STEVEN COLLEGE COLLABORATION — We use non-equilibrium molecular dynamics simulations to model stiffening mechanisms in viscoelastic polymer blends and nanocomposites with the overarching goal to understand the mechanisms for reversible thermal stiffening (stiffening while heating and softening up on cooling). The blend is comprised of two kinds of polymer chains with differing stiffness and glass transition temperatures (Tg) and the nanocomposite consists of nanoparticles grafted to the high Tg polymer phase in addition to the soft matrix phase. We employ both constant shear-rate and oscillatory shear deformations to characterize stiffening. Upon heating above the Tg of both polymeric phases, we show that significant stiffening arises due to the coupled relaxation and dynamics of both polymeric phases. The effects of shear rate, interaction strength between phases and the corresponding structural changes and dynamics leading to reversible stiffening are studied and are corroborated with experimental findings.

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