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MECHANICAL AND VISCOELASTIC PROPERTIES OF WRINKLED GRAPHENE REINFORCED POLYMER NANOCOMPOSITES – EFFECT OF INTERLAYER SLIDING WITHIN GRAPHENE SHEETS

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Multilayer graphene sheets (MLGS) are promising nano-reinforcements that can effectively enhance or tune the properties of polymer matrices. Despite many studies on MLGS reinforced polymer nanocomposites, the effect of wrinkles formed in MLGS on the reinforcement effect and viscoelastic properties of polymer nanocomposites has remained largely unknown. In this study, building upon previously developed coarse-grained models of both MLGS and polymethyl methacrylate (PMMA) coupled with molecular dynamics simulations, we have systematically investigated nanocomposites with different numbers of graphene layers and different wrinkle configurations. We find that with increasing waviness and decreasing number of layers, the elastic modulus of the nanocomposites decreases. Interestingly, we observe a sudden stress drop during shear deformation of specific wrinkled MLGS reinforced nanocomposites. We further conduct small amplitude oscillatory shear simulations on these nanocomposites and find that the nanocomposites with such wrinkle configuration also show peculiarly large loss tangent, indicating an increasing level of energy dissipation. These behaviors are attributed to the activation of the interlayer sliding among these wrinkled MLGS, as their interlayer shear strength is indeed lower than flat MLGS measured by steered molecular dynamics technique. Our study demonstrates that the viscoelastic properties of polymer nanocomposites can be tuned through wrinkle engineering of MLGS.

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