Structure and Mechanical Properties of Polymer-Grafted Nanoparticle Thin Films using Molecular Simulations

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Polymer nano thin films are quasi-two-dimensional materials with nanometer-scale thickness, currently being explored for applications in flexible electronics and drug delivery systems. Recent attention has shifted toward polymer nano thin films filled with nanoparticles (NPs), which offer the potential to achieve physical properties unattainable with conventional polymer films [1]. Among these, polymer-grafted nanoparticles (PGNPs) [2], which are surface-modified with polymer chains, are expected to enable the control of more complex self-assembled structures than those formed by traditional nanoparticles. However, the self-assembled structure and mechanical properties of PGNPs within the confined geometry of polymer nano thin films remain insufficiently understood. In this study, we employed coarse-grained molecular dynamics simulations to investigate the conditions required for superlattice formation within these thin films. Furthermore, we elucidated the relationship between the resulting self-assembled structures and the overall mechanical response of the system.
As a result, we identified the specific graft density and chain stiffness required to induce superlattice formation. Furthermore, we elucidated the mechanical mechanisms by analyzing the elastic modulus and the dynamic behavior of these self-assembled structures under uniaxial tension (Fig. 1).

Keywords:
Polymer nano thin film, Polymer nanocomposite, Polymer-grafted nanoparticle, Self-assembly, Molecular dynamics, Mechanical properties

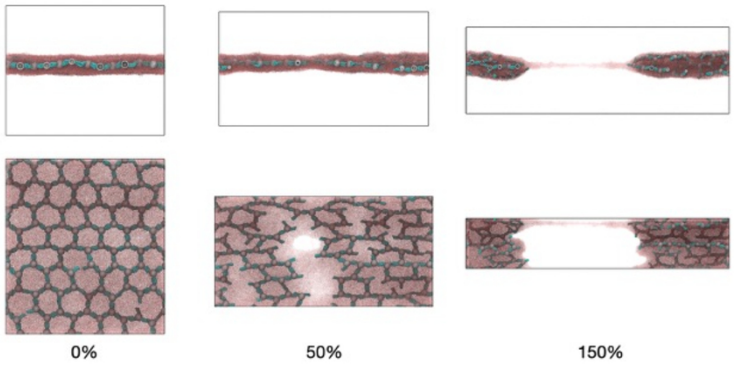

Figure 1. The snapshot of the systems before uniaxial tensile simulation (0%) and under uniaxial tensile simulation (50%, 150%)

References:

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