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How topological polymer loops on the nanoparticle surface control the mechanical properties of nanocomposites

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Carbon black (CB) and silica (SiO2) filled elastomers are known to be the most successful polymer nanocomposites (PNCs) in industry, where "bound rubber (BR)"(i.e., polymer chains that are physically or chemically adsorbed on the nanofiller surface) plays a critical role in their reinforcement. Here, we report a molecular-scale mechanism underlying the "BR-induced reinforcement"by integrating neutron scattering experiments and molecular dynamics simulations. Simplified non-crosslinked SiO2-filled polybutadiene (PB) and CB-filled PB reveal the critical role of topological polymer loops in the BR for the enhanced mechanical performance. The average loop size on the SiO2 surface modified with a silane coupling agent is much smaller than that on the CB surface and the loops on the SiO2 surface are densely formed, preventing interdigitation with the matrix chains. On the other hand, the larger, uncrowded loops formed on the CB surface facilitate the interdigitation with the matrix polymer chains even near the filler surface. In this way, a strong connectivity is established between a matrix and a nanofiller, resulting in an adhesive filler-polymer interface. Our findings shed light on rich and complex physics and materials design problems in PNCs, where the topological polymer structure on the nanofiller surface directly controls the macroscopic mechanical properties.

Topical Area

Soft matter: polymers, and complex fluids

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