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# Unravelling the Reinforcement Mechanism of Graphene–Thermoplastic Elastomer Composites through Experiments and Simulation

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**ABSTRACT**

Thermoplastic elastomers have attracted significant attention as sustainable alternatives to thermoset elastomers, owing to their reprocessability. Their adoption can reduce thermoset rubber waste in landfills and support more sustainable manufacturing practices. However, they generally exhibit inferior mechanical properties and durability compared to thermoset elastomers. Graphene-based nanomaterials (GNMs) have emerged as promising fillers in the rubber industry to achieve exceptional mechanical properties, and durability of an end product. The final performances of rubber nanocomposites are primarily governed by the nature and the strength of the interfacial interactions between the filler and the rubber matrix. In this study, we investigate the reinforcement mechanisms of thermoplastic elastomer styrene-butadiene-styrene (SBS) nanocomposites reinforced with 3 different 2D fillers; graphene nanoplatelets (GNPs), graphene oxide (GO), and reduced graphene oxide (rGO), spanning molecular-level interactions to macroscopic properties. Molecular dynamics (MD) simulations were employed to explore interfacial interactions, thermodynamic compatibility, and mechanical behaviour at the atomic scale. Experimentally, high shear melt mixing was used as a scalable, solvent-free processing method that overcomes the environmental and practical limitations of conventional solution blending. The effects of GNMs on mechanical, morphological, rheological, and thermal degradation properties were evaluated using tensile testing, scanning electron microscopy (SEM), atomic force microscopy (AFM), thermogravimetric analysis (TGA), and small angle neutron scattering (SAXS). Simulation results revealed strong interactions between

poly(butadiene) and graphene, leading to pseudo-crystalline ordering. GO exhibited the strongest affinity with poly(styrene), arising from π-π stacking and additional C=O … π and O-H … π interactions, correlating with the greatest enhancements in macroscopic tensile strength, modulus, and bound rubber content with improved elastic recovery. Furthermore, the study employed synchrotron macro-ATR-FTIR, a powerful technique that provides high-resolution chemical mapping and enables molecular-level insights into the interfacial interactions. AFM, SAXS and MD collectively revealed alterations in the SBS phase morphology, with GO preferentially interacting with the styrene phase. Rheological measurements showed lubricating effects in rGO-based nanocomposites at higher loadings. These fundamental insights offer a pathway toward designing lightweight, scalable, and reprocessable elastomer nanocomposites for advanced applications with the potential to replace thermoset rubbers.


**KEY WORDS**

Thermoplastic elastomers (TPEs), Styrene-butadiene-styrene (SBS), Elastomer nanocomposites, Graphene-based nanomaterials (GNMs), Interfacial interactions, Reinforcement mechanisms, Molecular dynamics (MD) simulations, Synchrotron ATR-FTIR, Sustainable, Reprocessable


**BIOGRAPHY**

Vihanga Kularatne is a third year PhD candidate in Chemical Engineering at RMIT University, Australia. His research focuses on thermoplastic elastomers and polymer nanocomposites, with an emphasis on their 3D printability for sustainable industrial applications. He has experience in both MD simulations and experimental synthesis and characterisation techniques. His work explores interfacial interactions and structure property relationships in elastomer systems. He aims to develop scalable, high performance, and environmentally friendly materials to replace conventional thermoset rubbers in advanced engineering applications, contributing to more sustainable and efficient manufacturing practices.

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