Multiscale modelling of the toughening mechanisms in rubber-toughened polymer nanocomposites: synergistic effect between different mechanisms

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ABSTRACT

As the design and scalable technology development of tough polymer nanocomposites without deterioration of stiffness receive attention in the automotive industry, fundamental understating of underlying toughening mechanisms at the nanoscale is inevitable. Mechanical tests on the rubber-toughened nanocomposites show that the overall fracture properties are much smaller than the reported theoretical predictions. Our previous analysis showed that major factors in this regard are the complex toughening mechanisms and the nano-structural features of the interface. As a result, “multiscale and multi-mechanism” modelling strategies may be necessary to take the contribution from each toughening mechanism into account.

We present, the effects of nanofibrillation (i.e., size, orientation, and dispersion) and interfacial tuning on the mechanical properties of nanofibrillated rubber-toughened nanocomposites using molecular dynamics (MD) simulations. Our aim is to demonstrate that by interfacial modification via grafting compatibilizer at the interface, nanofibrillated rubber-toughened polypropylene (PP) nanocomposite can achieve superior mechanical properties as a result of enhanced interfacial load transfer. Compared to pure ethylene propylene diene monomer rubber (EPDM)/PP system, an increase of 49% in energy absorbed per unit volume during fracture was achieved for 30% functionalized nanocomposites. Such an increase in energy dissipation was caused by a transition in the dominant crack propagation mechanism from interfacial slippage to crack-arresting behavior, owing to enhanced interfacial adhesion. MD simulations in conjunction with the multiscale model revealed that such a change in mechanism is caused by the formation of strong covalent bonds, interfacial friction, and the presence of a highly entangled polymeric network at the interface.

We also present that the synergism (e.g., coupling effect) exists when different mechanisms across bridging and process zones operate simultaneously. This considerably enhances the toughness even larger than the summation of enhanced energy dissipation for each mechanism. Furthermore, deleterious interactions are also considered to quantify the threshold value of EPDM content for such interactions. While the multiscale framework can be considered as a roadmap for modelling the interface for different nanocomposite systems, the obtained results may provide useful insights for the robust and scalable fabrication of nanofibrillated rubber-toughened nanocomposite structures which is technologically challenging.