Editorial corner – a personal view

Proper molecular level tool to explore the structure-property relationships in elastomer nanocomposites

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Establishing a quantitative relation between the structure and properties of elastomer nanocomposites (ENCs) is still challenging and requires the multi-scale approach. To clearly and comprehensively characterize the multi-scale structure of ENCs, molecular dynamics simulation proved to be a powerful tool. We have studied the dispersion of nanoparticles (NPs) with different shapes in the elastomer matrix (DOI: [10.1021/la201073m](https://doi.org/10.1021/la201073m), DOI: [10.1016/j.polymer.2014.01.042](https://doi.org/10.1016/j.polymer.2014.01.042)), and the interfacial chain mobility nearby the NPs (DOI: [10.1039/c0cp02952a](https://doi.org/10.1039/c0cp02952a)). One important finding is that polymer depletion induces direct aggregation of NPs at low rubber-NPs interaction and at high interfacial interaction NPs are bridged via polymer chains, between which NPs exhibit a homogeneous dispersion by adsorbing a layer of polymer chains. This simulation result is consistent with the theoretical prediction (DOI: [10.1021/ma060577m](https://doi.org/10.1021/ma060577m)).

Besides the molecular level characterization, the static and dynamic mechanical properties are also investigated. We have examined the reinforcement mechanism due to spherical and rod-like NPs (DOI: [10.1039/c4cp01555j](https://doi.org/10.1039/c4cp01555j), DOI: [10.1039/c0cp00297f](https://doi.org/10.1039/c0cp00297f)). It was found the destruction of the network formed by aggregation between NPs directly or NPs via bridged polymer chains leads to the occurrence of the Payne effect under external tensile or shear loading (DOI: [10.1039/c4sm00233d](https://doi.org/10.1039/c4sm00233d)). Since ENCs always exhibit

strong viscous loss attributed to the large internal friction between various structural units, we design a compounding system by mixing elastomer with carbon nanosprings, which are a kind of helical carbon nanotubes and possess reversible mechanical deformation, and we find the hysteresis loss during the tension-recovery process can be dramatically reduced by enhancing the interfacial interaction between elastomer and carbon nanosprings and the spring constant of carbon nanosprings. This may open a new avenue for the fabrication of automobile tires made of ENCs with low fuel consumption (DOI: [10.1002/adfm.201201438](https://doi.org/10.1002/adfm.201201438)). Based on these research works, it is believed that molecular dynamics simulation will play an important role in the study of ENCs. However, future progress should be focused on improving the simulated realness to come close to the experimental systems as much as possible, and increasing the calculation speed to cover multi-scale and length, which need and deserve more scientists to devote their efforts.

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