Editorial corner – a personal view

Quantitatively predicting the structural and mechanical properties of elastomer nanocomposites via molecular dynamics simulation

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Accurately and quantitatively predicting the properties has been a long-standing challenge in exploring the structure-property of elastomer nanocomposites (ENCs) and designing materials without experiment. Among various methods, molecular dynamics (MD) simulation is convincing in characterizing the multi-scale structure of ENCs, especially the dispersion of nanoparticles (NPs), chain and NP mobility, and interfacial properties (<https://doi.org/10.3144/expresspolymlett.2015.54>). Non-equilibrium MD simulation has been used in calculating the static and dynamic mechanical properties of ENCs using various models. To achieve accurate characterizations, fully atomistic/optimized coarse-grained models and accurate forcefields are essential, which have been validated successfully in quantitative calculation of structural properties, *e.g.* glass transition temperature (<https://doi.org/10.1021/acs.macromol.0c01285>) and solubility parameter (<https://doi.org/10.1039/c8ra00572a>). However, limited by relatively small length scale of the system and short simulation time scale, the mechanical response usually exhibits too high stress values, prohibiting the access to accurate structure-mechanical property values.

Stress-strain (SS) relation, produced by the uniaxial deformation, is one of the most concerned characterizations of the static mechanical properties. Reducing the strain rate (<https://doi.org/10.3390/nano9081088>) is necessary but costly. It is validated that the stepwise

deformation and relaxation method (<https://doi.org/10.1016/j.polymer.2019.03.006>), allowing the polymer chain to relax between stepwise deformation, is efficient in obtaining the SS curve analogous to experimental values. Besides, combining the MD simulation with the quasi-static field (<https://doi.org/10.1021/acs.macromol.5b01236>), the multiscale method, is also an alternative to calculate the static mechanical properties of polymer. In addition, based on the SS curves performed by simulations with high strain rates, predicting the SS relation under low strain rate via a neural network has been proposed (<https://doi.org/10.1109/ICNSC48988.2020.9238085>).

An even more complex case is the simulation of the dynamic mechanical property, obtained under oscillatory deformation (<https://doi.org/10.1039/c7cp02945d>). We have qualitatively elucidated the non-linear behavior of ENCs (<https://doi.org/10.1039/c4sm00233d>). However, due to the high frequency of strain, obtaining the accurate storage/loss modulus and loss factor of ENCs still needs more efforts. It could be achieved by employing time-temperature superposition and improving the computing efficiency with a coarse-grained model (<https://doi.org/10.1002/polb.23976>) in the future.

In conclusion, we anticipate that the MD simulation will provide convincing results in the prediction of structure-mechanical property of ENCs, in parallel with the experimental research.

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