Molecular dynamics simulation of polymer nanocomposites: current achievements and future opportunities

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Abstract

Besides experiment and theory, computer modeling and simulation has already become the third important research approach, because of its unique advantages such as convenience and intuition. In this talk I will systematically introduce research achievements of polymer nanocomposites (PNCs) through molecular dynamics simulation, carried out in our research group. First, we studied the dispersion and aggregation behavior of bare nanoparticles (NPs) with different geometries such as spherical, sheet-like and rod-like under quiescent and shear cases. To model small ligands used in experiments to realize better dispersion, we investigated the dispersion of NPs end-grafted with polymer chains by varying the grafted chain length and grafting density. Second, we probed the translational and relaxation dynamics at the chain and segmental length scales of the interfacial regions, hoping to elucidate whether “glassy layers” exist around NPs. Third, we simulated the enhancement of the Young’s modulus, stress-strain and fracture toughness induced by NPs, providing a molecular reinforcing mechanism. Fourth, the famous “Payne effect”, namely the decrease of the storage modulus as a function of the strain amplitude was examined, uncovering the underlying reason responsible for this non-linear behavior, and how the introduced carbon nano-springs can effectively reduce the dynamic hysteresis of PNCs is as well illustrated. Fifth, we also simulated the formation of conductive network. Lastly, future simulation challenges and opportunities of PNCs are presented. In general, computer modeling and simulation is shown to have the capability to obtain some fundamental understanding of PNCs at the molecular level, in hopes of providing some design basis and principles for synthesizing and preparing multi-functional and high performance PNCs.

References

2. Jun Liu, Liqun Zhang³, Dapeng Cao, Jianxiang Shen, yangyang Gao; Computational simulation of elastomer nanocomposites: current progress and future challenges; Rubber Chemistry and Technology; 85, 450-481(2012). (An invited review)
Short Biography

Jun Liu is an associate professor in the department of Materials Science and Engineering of Beijing University of Chemical Technology, and he mainly focuses on simulating the structure, dynamics, static and dynamic mechanical properties of polymer nanocomposites through molecular dynamics simulation. He has published over nearly twenty peer reviewed papers, such as Advanced Functional Materials, Macromolecules, Soft Matter, Langmuir and so on.