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Aggregation on the Study of Tribological Properties of Polymer Composites: Molecular Dynamics Simulations

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Abstract

In this study, a brief review of the molecular dynamic's simulations application in research of tribological properties of polymer composites were presented. To better classify and aggregate, particular attention is given to the frictional factor analysis and the enhancement of polymer composites on the tribological properties. The review of the latest research progress of the tribological research by molecular dynamics simulations and some proposals for further research may have implications for the relevant research and applications, which is practically meaningful and helpful for the related researchers to have a better understanding of this field.

Keywords: Molecular Dynamics Simulation; Polymer Composites; Tribological Properties

Introduction

Polymer composites are widely applied in various aspects of scientific and engineering applications, such as industrial production, petrochemicals, automotive industry, military, aeronautics and astronautics, and daily life owing to some of their excellent properties such as wear and corrosion resistance [1,2]. In particular, some important components often face severe working conditions such as high temperature and pressure, corrosion, swelling, and abrasive wear et al. [3,4]. Researchers have done a lot to improve the properties of polymer composites. As is known, simulation has become one of the important methods to study the properties of materials with the development of computer technology. Molecular dynamics simulations have been recognized and widely used due to the unique microscopic perspective as a new simulation method in recent years [5]. As an important index to characterize polymer composites, tribological properties are also one of the key research contents of molecular dynamics simulations. Therefore, many researchers are committed to the research of tribological properties by molecular dynamics simulation.

Discussion

Factor Analysis

The influencing factor analysis of the tribological systems by molecular dynamics methods are first aggregated. Kreer et al. [6] studied the tribological properties of two polymer brushes at different relative sliding speeds. It is found that the lateral force between the polymer brushes decreases logarithmically with an increase in the relative sliding speed v0 in a range that is more than ten times V_0. Li et al. [7] developed three-layer molecular frictional pair models between Fe atoms and polymer/carbon nanotube composite to study the friction coefficient and wear rate with different sliding speed of iron nanorods. The results show that the friction coefficient and wear rate of CNT / polymer composites are reduced from 0.356 to 0.322 and 26% -6% at sliding speeds of 0.01 to 0.11 Å / ps. Heo et al. [8] studied the effect of sliding orientation on the tribological properties of polyethylene (PE) by using classical molecular dynamics simulations. The results show that the friction coefficient of sliding in the parallel direction is smaller than that of sliding in the vertical direction. Yuan et al. [9] studied the effect of scratch speed on nano scratching behavior. It was found that when the local temperature in the scratch region exceeds the glass transition temperature Tg, the polymer material in the scratch region around the indenter is removed in a tough manner. Larger scraping rates result in more material deformation and higher pile-up. For larger scraping speeds, the tangential and normal forces are larger, and the coefficient of friction is almost independent of the scraping speeds studied.

Lubrication condition during friction is also one of the focuses of tribology research. Braun et al. [10] used a simple two-dimensional model to study the rolling of spherical lubricant

molecules' effect on the friction system. Molecular dynamics simulations show that the rolling of spherical lubricant molecules exists only when the concentration is lower than that of the close-packed layer. Dai et al. [11] used molecular dynamics simulations to analyze the lubrication effect of perfluoropolyether (PFPE) films to reveal the mechanism behind the interface lubrication behavior of nanoelectromechanical (NEMS) systems and understand the performance of the films. The study found that due to the linear fluidity of the PFPE film, it can promote surface reconstruction and provide good lubricity. The simulation results match the experimental characterization well. Berro et al. [12] used molecular dynamics simulations to study the tribological properties of lubricant mixtures containing cetane base oil and 5% zinc dithiophosphate (ZDDP) under molecular confinement constraints. The results show that mechanical and thermal slip can be reduced by increasing the surface energy. Compared with pure cetane, the migration of ZDDP molecules and their adsorption on solid surfaces can significantly inhibit mechanical slip and leading to an increase in friction coefficient.

Material enhancement

To improve the tribological properties of polymer composites, MD simulations also involve studying from atomic views. Li et al. [13] established and studied a three-layer molecular model that contains Fe atoms as the top and bottom layers and uses the nitrile-butadiene rubber and carbon nanotube matrix as the core to understanding how to improve nitrile-butadiene rubber composition by incorporating carbon nanotubes as a reinforcing agent. Chawla [14] Developed graphene-reinforced natural rubber composites to study the improvement of mechanical and tribological properties of natural rubber by introducing graphene as a reinforcing material. The results show that after strengthening natural rubber with a single-layer graphene oxide sheet, Young's modulus increased by 185%, the shear modulus increased by 32%, and the hardness increased by 48%. Moreover, the friction coefficient and wear rate obtained by introducing graphene oxide sheets in the natural rubber matrix were reduced by 28% and 36%. He et al. [15] used molecular dynamics simulations to study the enhanced tribological properties of polymer / nano-SiO_2 composites by sliding a top iron layer on the surface of the polymer composite. The results show that by introducing nano-SiO_2 particles, Young's modulus is increased by about 190%. The average friction coefficient and wear rate of the polymer / nano-SiO_2 composites were reduced by approximately 27% and 47.4%, respectively. Li et al. [16] established a molecular model with Fe atoms as the top nanorods and the bottom layer and a polymer/carbon nanotube composite as the core to check the friction by sliding the top Fe nanorods on the surface of a polymer matrix under normal load coefficient and wear rate. Simulation results show that by introducing carbon nanotubes, the average friction coefficient of the composite material is reduced by about 38%, and the average wear rate is reduced by 60%. Chawla et al. [17] used molecular dynamics simulations to study Young's modulus and tribological properties of pure styrene-butadiene rubber (SBR) polymers and carbon nanotube-reinforced polymer composites. The mechanism of using CNTs to enhance friction performance was studied and discussed. When carbon nanotubes are used as the reinforcing material, the obtained Young's modulus indicates that the mechanical properties of the SBR polymer are improved.

Conclusion

Molecular dynamics has been widely used in the study of tribological properties of polymer composites for its excellent advantages. However, due to the large amount of calculation and the small calculation scale, the limitations of large calculation time, fluctuation in results and the susceptibility to size effects cannot be ignored. In the foreseeable future, the research on the mesoscopic scale, the improvement of atomic-scale research methods and the combination with macro-scale simulation methods will be some areas worth further exploration for the molecular dynamics study of the polymer composites on the tribological and some other properties. The contribution of this study is expected to broaden the research area of molecular dynamics and conduct a more thorough and comprehensive study of rubber materials.

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