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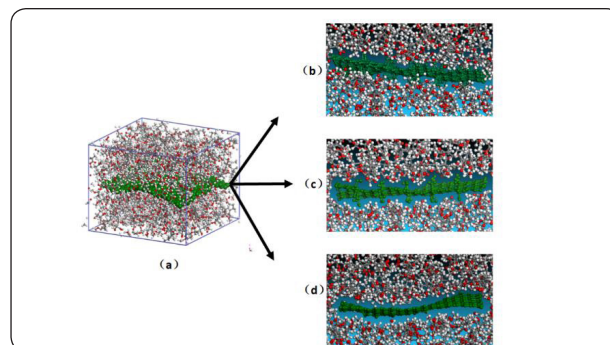
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Molecular dynamics simulations of mechanical and tribological properties of polymer composites enhanced by cross-linked graphene sheets

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Molecular models of polymer composites reinforced by pristine, functionalized and cross-linked graphene are developed to compare the enhancement of mechanical and tribological properties of polymer composites via molecular dynamics simulations. Constant strain method is applied to calculate the elastic behaviors of the polymer composites. The results show that about 54.2% and 19.3% higher in Young's modulus, 60.8 % and 26.9 higher in tensile strength are obtained for the composites by incorporation of cross-linked graphene than those by incorporation of pristine and functionalized graphene. Moreover, three-layer molecular model containing Fe atoms as the top and bottom layers and polymer and graphene matrix as the core is built to compare the improved tribology properties of the polymer composites by incorporation between functionalized and cross-linked graphene as the reinforcements. The simulation results show that decreases of about 13% and 42.3% in the average friction coefficient and abrasion rate of the cross-linked graphene/polymer composites can be achieved. In order to reveal the mechanisms of the findings, the interfacial interaction energy, RDF values between carbon nanotubes and polymer matrix, et al. are particularly calculated and explained.



Recent Publications

1. Li, Y., Wang, S., Arash, B., & Wang, Q. (2016). A study on tribology of nitrile-butadiene rubber composites by incorporation of carbon nanotubes: Molecular dynamics simulations. *Carbon*, 100, 145-150.
2. Li, Y., Wang, S., Wang, Q., & Xing, M. (2016). Molecular dynamics simulations of tribology properties of NBR (Nitrile-Butadiene Rubber)/carbon nanotube composites. *Composites Part B: Engineering*, 97, 62-67.
3. Li, Y., Wang, S., He, E., & Wang, Q. (2016). The effect of sliding velocity on the tribology properties of polymer/carbon nanotube composites. *Carbon*, 106, 106-109.
4. Li Y, Wang S, Wang Q. A molecular dynamics simulation study on enhancement of mechanical and tribological properties of polymer composites by introduction of graphene. *Carbon*, 2017, 111:538-545.
5. Li Y, Wang S, Wang Q. Enhancement of tribological properties of polymer composites reinforced by functionalized graphene. *Composites Part B: Engineering*, 2017, 120:83-91.

Biography

Mr. Li is a Ph. D. Student in Shenyang University of Technology. He used to be an exchange student in Aalen University, Germany, and visitor in City University of Hong Kong and Southern University of Science and Technology. His academic aspects are related to mechanical and tribological properties of polymer nano-composites and nanotechnology. He has published some scientific papers on renowned journals, such as "Carbon", "Composites part b: engineering". He was awarded the "National scholarship" in 2017 and 2016 respectively.

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