ICCES, 2023, vol.26, no.3
DOI: 10.32604/icces.2023.09070

PROCEEDINGS

Molecular Dynamic Study on Entangled Structure of Polymer Chains' Network under High Speed Loading Condition

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ABSTRACT

It is well known that the mechanical resistance of soft materials such as rubber and elastomer can be improved by cross-linkages or fillers, which will lead to a construction of entangled structure of polymer chains' network. However, the correlation between the amount of cross-linkages or fillers with the toughness strength of the resultant material has not been clarified. Therefore, in this study, we at first construct a computational model for the resultant material with molecular dynamics method. Then, a series of simulations are performed for the resultant materials with different amount of cross-linkages or fillers under high speed loading condition. Finally, the development of entangled structure of polymer chains' network is investigated and the effect of such development on the toughness strength of soft materials is evaluated. The results show that even though the increase of the amount of cross-linkages leads to the increase of the mechanical resistance, the development of the average radius of gyration of polymer chains is suppressed. As a result, the relative movement of polymer chains is limited in the soft material with large amount of cross-linkages and the toughness strength decreases eventually. With regard to the effects of speed of loading on the development of entangled structure of polymer chain's network as well as the toughness strength of soft materials, we will show them in our full paper.

KEYWORDS

Molecular dynamics method; polymer chain's network; entangled structure; toughness strength

Funding Statement: The authors received no specific funding for this study.

Conflicts of Interest: The authors declare that they have no conflicts of interest to report regarding the present study.

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