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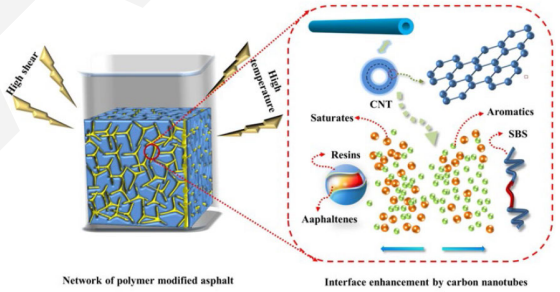
Molecular dynamics simulation and microscopic observation of compatibility and interphase of composited polymer modified asphalt with carbon nanotubes

Key words: Polymer modified asphalt; Carbon nanotubes; Molecular dynamics; Microstructure characteristics; Interphase enhancement

- Interfacing and compatibility are the most challenging issues that affect the performance of polymer modified asphalt.

- Although the current theory can qualitatively describe the influence of modifiers on asphalt, the microscopic mechanism has not been well studied.

- There have been some reports on molecular dynamics, however, there is still a limited understanding of the macroscopic properties of asphalt materials by molecular dynamics simulation.

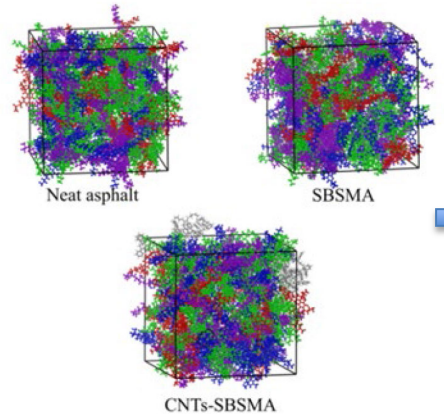


- Herein, we report a molecular dynamic simulation method to simulate the self-assembly behavior of SBS-modified asphalt and CNTs/SBS-modified asphalt systems.

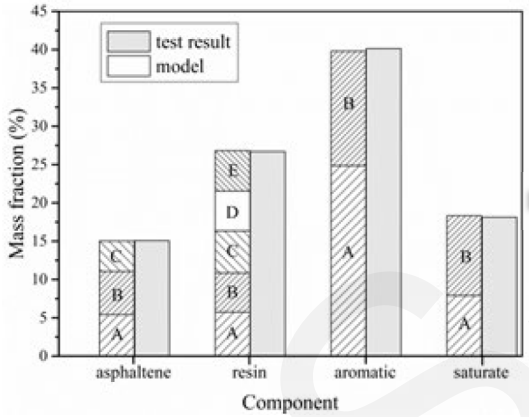
- The aim of this study is construct a bridge between the microstructure and the macroscopic properties of SBS-modified asphalt, thereby revealing the microscopic mechanisms of modified asphalt.

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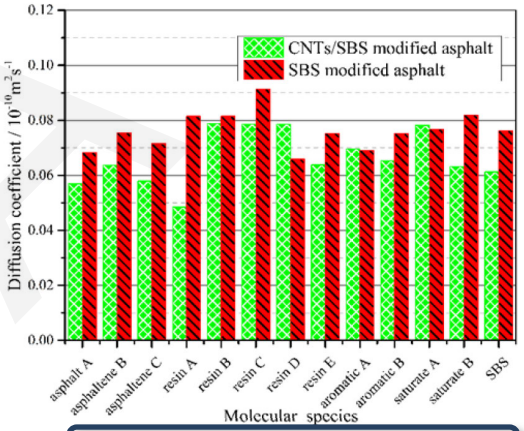
METHOD



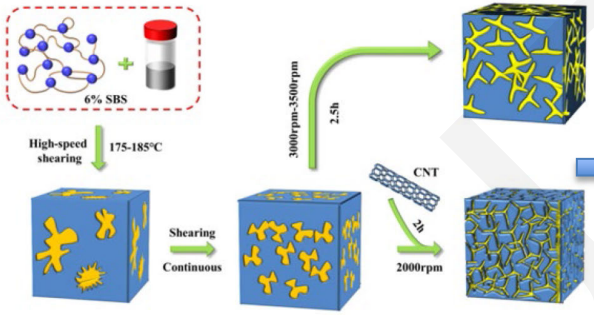
Models



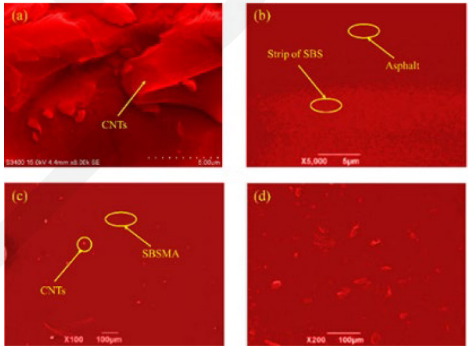
Validation



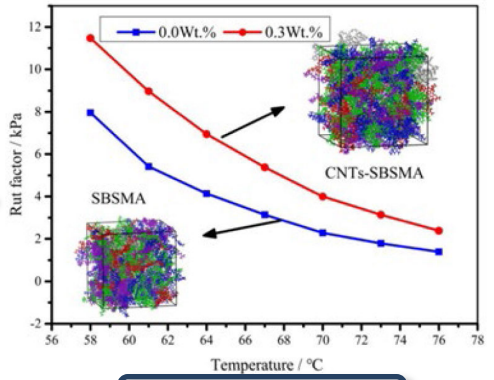
Molecular dynamic simulation



Preparation of samples



Micromorphology



Rutting factors

RESULTS AND CONLUSIONS

- The addition of CNTs greatly increased the binding energy of various molecules in asphalt with SBS polymers, which made the SBS-modified asphalt system more stable. The morphology of the interaction between SBS and asphalt was further analyzed and the compatibility of SBS with aromatics and saturates was found to be high as the molecules intertwined with each other. However, asphaltenes are also intertwined with aromatics and saturates, indicating that SBS will compete with asphaltenes for these light components in the asphalt system, which may result in inadequate SBS swelling.

- A t test was performed on the binding energy of the two modified asphalt systems, and it was found that both data sets are a normal distribution, and the difference between them is not statistically significant. This means that CNTs did not impact the weak interaction between SBS and asphalt.

- The MSD curves of various molecules in the two systems were obtained and their diffusion coefficients were calculated. It was found that CNTs decreased the diffusion coefficients of each molecule in the asphalt systems. The correlation coefficient between the diffusion coefficient with the molecular weight, surface area, and volume were calculated, and it was found that CNTs increased the absolute value of the correlation coefficient. However, the correlation with molecular weight, surface area, and volume were still low, less than 0.3, indicating that the diffusion of various molecules in the asphalt system was not significantly affected by surface area, molecular weight, or volume, but mainly depends on the interaction between molecules in the system.

- Relative concentration distribution curves were analyzed to verify the colloid structure theory that SBS will compete with asphaltenes for aromatics and saturates. The competition is fierce; however, the addition of CNTs makes the distribution of aromatics and saturates more uniform, alleviating the competition between SBS and asphaltenes, thereby promoting the swelling of SBS. Thus, CNTs inhibited the diffusion of various molecules in the system but guided the movement of various molecules in the system, thereby increasing the stability of the system.

RESULTS AND CONLUSIONS

- Samples of SBS-modified asphalt and CNTs/SBS-modified asphalt were prepared and a rut test was conducted. CNTs were found to enhance the rut factor of SBS-modified asphalt at various temperatures (growth was between 44.1% and 75.4%). The microscopic morphology of SBS-modified asphalt and CNTs/SBS-modified asphalt samples were observed using a SEM. CNTs caused the SBS distribution to be more uniform and the SBS polymers to fully swell. SEM and fluorescence microscope were used to observe the micro-morphologies of the two systems, which matched well with the molecular dynamics simulation results. The experimental results agree well with the simulation indicating that the molecular dynamics simulation of the self-assembly of SBS-modified asphalt in this paper is reliable.

- The difficulty in studying modified asphalt is that it is an extremely complex system, containing millions of molecules and various impurities, and the composition of asphalt from different sources is wildly different. Therefore, even after many researchers have studied asphalt, there is no universal law. The limitation of this study is that twelve kinds of molecules are used to represent the asphalt system. Although twelve is more complex than asphalt models constructed by other studies, it is still far from accurately representing the complexity and randomness of asphalt. There is an opportunity for further development of this complex system by chemists.

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