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Review

Performance characteristics of asphalt materials based on molecular dynamics simulation – A review

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HIGHLIGHTS

- Molecule dynamic simulation method is found to act as an applicable tool in asphalt materials.
- Molecule dynamic simulation bridges the gap between macro and micro scope behaviors.
- Interface properties could be evaluated by molecule dynamic simulation.
- An accurate molecular structure is the foundation of molecule dynamic simulation.
- Computer science and molecular model development will widen application of molecule dynamic simulation.

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ABSTRACT

Molecular simulation method has been widely applied to various fields with the rapid development of computational techniques. Molecular dynamics (MD) simulation applications in asphalt material were introduced in this paper. Procedures of conducting MD simulation and significant parameters were illustrated and promotions of asphalt molecular model were summarized to get a better results in further simulation. Asphalt mechanical properties, interactions between various fractions, diffusion behaviors, and effects of aging and modifier investigated by MD simulation were presented. Interface properties of asphalt/aggregate including adhesion and mechanical effect of moisture on interface were efficiently predicted by MD simulation. The review results indicated that MD simulation method was found to act as an applicable tool to predict the performances of asphalt materials and bridge the gap between macro and micro scope behaviors. This technique significantly help understand MD simulation application characteristics in asphalt materials including adhesion, cohesion, diffusion, and engineering prediction in terms of the effects of several factors and give insights to a wide usage of MD simulation in the future.

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1. Introduction

Asphalt binder has been widely used as a construction material in road and highway pavement over past several decades [1]. During these years, a high quality asphalt pavement is constantly required to fulfill more requirements for prolonging its service life. A myriad of research studies were completed to investigate the properties of asphalt binder since it directly affected performance of asphalt pavement [2–5]. Asphalt binder is a composite and multiscale material characterized by the size of its composition. The inner structure of asphalt material can be analyzed from macro, meso and micro scales [6], as shown in Fig. 1. Macro performance of asphalt binder was found to be determined by its micro structure and explained by its micro mechanisms, while the existing experimental methods for asphalt binder are mainly conducted from macro perspective and unable to capture the intrinsic changes attributed to some kinds of failures [7]. With the development of research techniques, a growing number of micro approaches became effective to predict the macro performance of material. For example, molecular dynamics (MD) simulation is one common type of these methods. It can be applied to analyze sorts of molecular systems at gas, liquid and solid phases. Some issues related to big molecule, high polymer molecule and biochemical molecule can also be solved in this way.

Molecular dynamics simulation is a computational method based on statistical mechanics and thermodynamics theory to simulate the interactions and behaviors of various atoms and molecules under certain conditions. Meanwhile, the chemophysical properties and thermodynamics characteristic of a molecular system can be obtained after simulation. According to this method, an precision molecular structure is conducted firstly so as to show the geometry of molecules accurately and then a proper force, known as an equation, described potential energy is set to insure the interactions between atoms and surrounding molecules reasonable. And thus dynamic behaviors of every single molecule can be determined under certain ensemble, referring to a set of identical conditions such as temperature, volume and pressure. Molecular dynamics simulation was firstly adopted by Alder and Wainwright to investigate the equilibrium state equation of liquid and solid in 1957 [8]. Researchers such as Verlet, Anderson, Nose and Hooverd have made great contributions on molecular dynamics simulation since 1970s so that widened its application [9–11]. Two particular purposes of molecular dynamics simulation are to achieve prediction of material behavior and explanation of mechanism, referring to predict the macro performance of a material and optimize the synthesis process, with the purpose of producing a new material, and give mechanism illustration about some experimental results which are hard to be explained by current existing methods.

Molecular dynamics simulation has been widely used in the field of biochemistry to deal with the issues of equilibrium and nonequilibrium states as well. As for the behavior of polymer

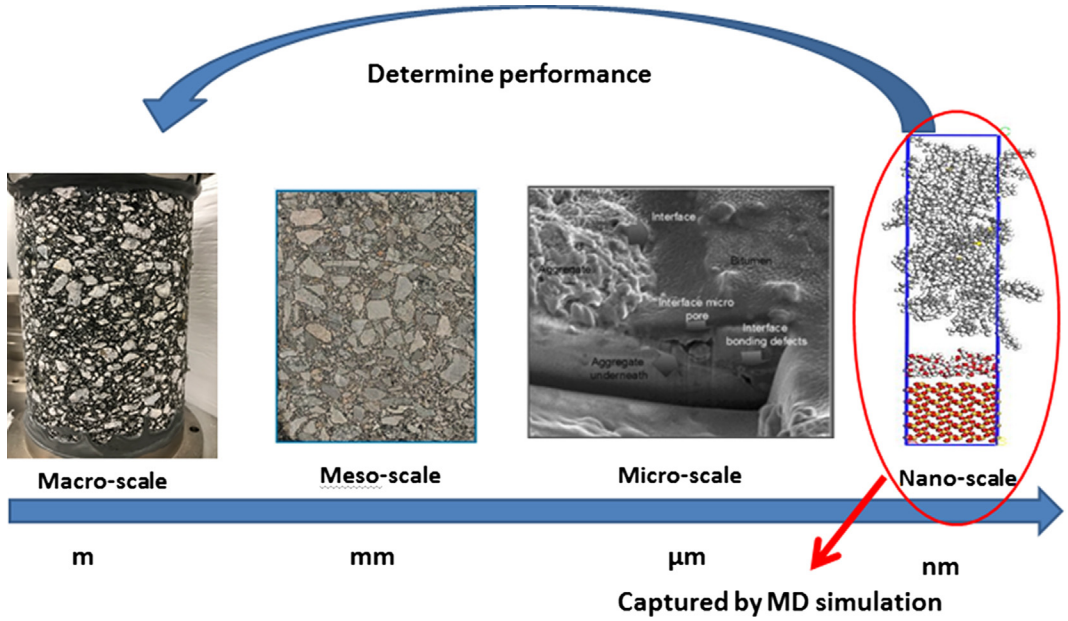

Fig. 1. Multiscale of asphalt materials.

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