Molecular scale analysis of the properties and toughening mechanism of polyethylene glycol modified epoxy asphalt

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Abstract：Polyethylene glycol（PEG）with different chains was used to modify epoxy asphalt. Molecular models of PEG-modified epoxy asphalt were developed using molecular simulations（MS）. The thermodynamic and mechanical properties of PEG-modified epoxy asphalt were analyzed, and its toughening mechanisms were explored. A method based on the Dijkstra algorithm was proposed to evaluate epoxy asphalt crosslinked networks. The results show that the introduction of PEG chains into epoxy asphalt can lower the glass transition temperature and enhance its toughness because of the extended length of the PEG chains, which can increase the free volume and improve the mobility of the epoxy resin in the epoxy asphalt. The crosslinked network quantitative evaluation method based on the Dijkstra algorithm can effectively evaluate the distribution of epoxy asphalt crosslinking bonds, providing further explanation of the toughening mechanism of PEG-modified epoxy asphalt. The feasibility of designing and screening epoxy asphalt materials by MS is verified, and a guide for toughening mechanism research of epoxy asphalt at the molecular level is provided.
Key words：molecular simulation; crosslinked epoxy asphalt; thermodynamic properties; mechanical properties; toughening mechanism
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Epoxy asphalt, a thermosetting material, comprises epoxy resin, curing agent, asphalt, and other additives[1-2]. It possesses the characteristics of high temperature stability, strong adhesion, and excellent fatigue resistance, which makes it a popular choice for various applications such as pavements, bridge decks, and airport runways. Bisphenol A epoxy resin（DGEBA）is a commonly used resin for preparing epoxy asphalt. However, the rigid nature of DGEBA contributes to material brittleness and lack of ductility, which limits its use in advanced applications[3]. To enhance its usability, the flexibility of epoxy asphalt requires considerable enhancement through modification.

Many methods are available to enhance the toughness of epoxy asphalt. The toughness of epoxy asphalt can be improved by incorporating modifiers such as rubbers, fibers, and nanomaterials[4-5]. However, this method results in increased viscosity of epoxy asphalt, thereby reducing the time available for construction. The mobility of an epoxy asphalt network structure can be enhanced by incorporating external plasticizers, including o-phthalic anhydride methyl ester, ethyl ester, and similar materials[6-7]. However, the migration of external plasticizers to the material surface and subsequent volatilization into the surrounding environment can cause environmental pollution and reduce the performance of epoxy asphalt.

Incorporating reactive agents or tougheners into an epoxy resin or curing agent is an ideal approach. In general, reactive agents can consist of repeating units such as —C— C—C—, —C—O—C—, and —C—Si—C—[6]. These agents chemically react with epoxy during curing, forming a tough and flexible network. Polyethylene glycol（PEG）, which contains C—O—C bonds, is a good choice for toughening epoxy asphalt. The flexible molecular chains of PEG can help reduce stress concentration and absorb impact energy, thereby reducing the brittleness of epoxy asphalt[8].

The effects of PEG addition on the microstructure and macroscopic properties of epoxy asphalt and its modification mechanism can be explored through experimental tests, which are always criticized as costly and inefficient. In contrast, molecular simulation（MS）combines theoretical methods and computer technology to simulate molecular motions[9-10]. This method effectively illustrates how a microstructure influences the macroscopic properties of epoxy asphalt, thereby saving time and avoiding material waste[11-12].

In the present study, different PEG chains were considered to toughen epoxy asphalt. MS was employed to investigate the thermodynamic and mechanical properties of epoxy asphalt modified with PEG. In addition, the toughening mechanism of PEG-modified epoxy asphalt was discussed from the molecular perspective.

1 Molecular Model Construction and Crosslinking Reaction

1.1 Molecular models

1.1.1 Molecular model for curing agent and epoxy resin and curing agent

The epoxy asphalt consisted of epoxy resin, curing agent, and asphalt. The epoxy resin was DGEBA with an epoxy equivalent of 196.1. Tung oil anhydride (TOA) was used as the curing agent. Different PEG chains with molecular weights of 200, 400, and 800 were employed to react with TOA in order to toughen the epoxy asphalt. The ratios of TOA and PEG with the three different molecular weights were set to 4:1, 2:1, and 1:1, respectively. The molecular structures of DGEBA, TOA, and

PEG are shown in Fig. 1. PEG reacted with TOA to form a new curing agent that contained a long-chain polyether, which was then crosslinked with DGEBA. This reaction process is shown in detail in Fig. 2.
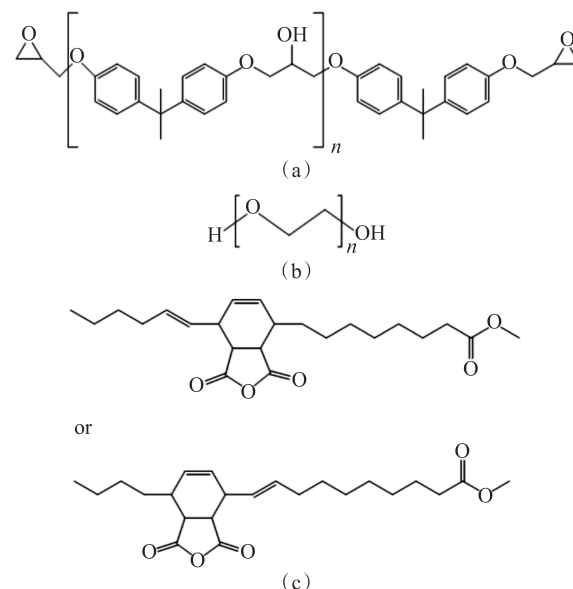

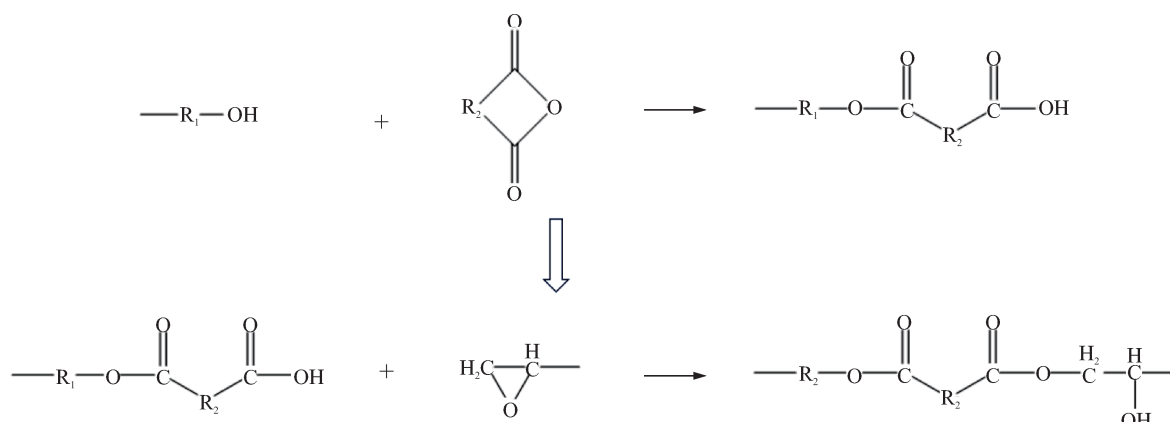**Fig. 1** Molecular structures. (a) DGEBA; (b) PEG; (c) TOA

Fig. 2 Reaction process of the curing agents and epoxy resin

1.1.2 Molecular model for base asphalt

In the current study, 70# asphalt was selected as one of the components of the epoxy asphalt. During the modeling process, it is necessary to ensure that the constructed model closely matched the 70# asphalt sample in terms of four components, elemental composition, and molecular weight. On the basis of previous research, the representative molecules shown in Fig. 3 were selected to construct the asphalt molecular model[13-14]. Table 1 lists the detailed information about the four components of the 70# asphalt.

1.2 Construction of precrosslinking model

In the current study, the Amorphous Cell module of Materials Studio was used to build precrosslinking amorphous three-dimensional (3D) models of epoxy resin,
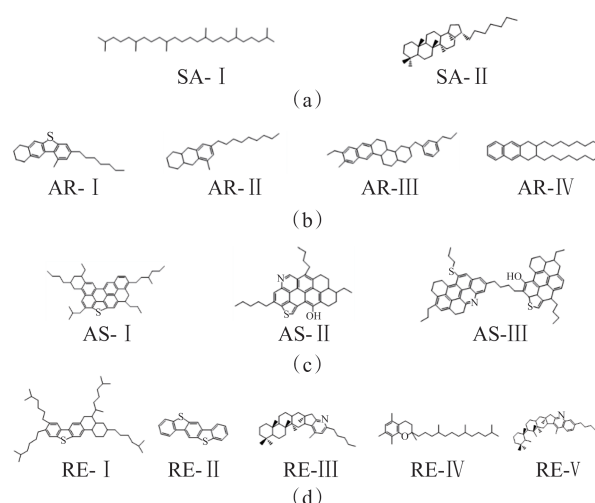

Fig. 3 Molecular structures of 70# asphalt. (a) Saturate; (b) Aromatics; (c) Asphaltene; (d) Resin
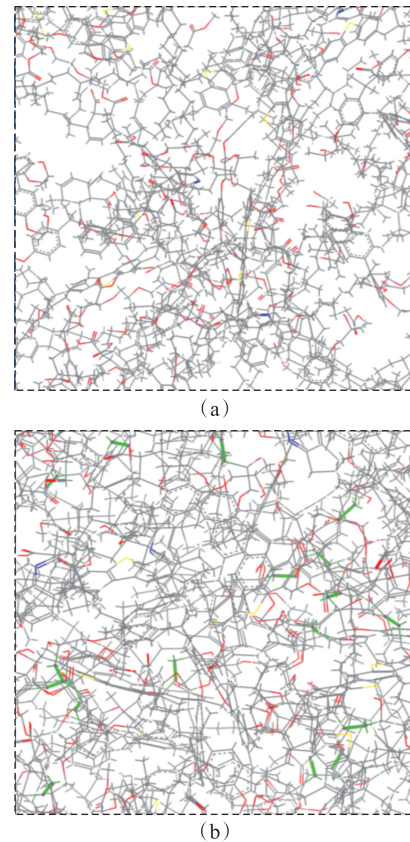
Table 1 Detailed information on the four components of the asphalt models

Component	Molecular label	Chemical formula	Molecular weight	Number
Saturate	SA-I	$C_{30}H_{62}$	422.826	3
	SA-II	$C_{35}H_{62}$	482.881	4
Aromatics	AR-I	$C_{24}H_{30}S$	350.564	12
	AR-II	$C_{24}H_{38}$	326.568	6
	AR-III	$C_{35}H_{44}$	464.737	6
	AR-IV	$C_{30}H_{46}$	406.698	7
Asphaltene	AS-I	$C_{50}H_{60}S$	693.09	3
	AS-II	$C_{36}H_{39}NOS$	533.774	1
	AS-III	$C_{63}H_{65}NOS_2$	916.339	1
Resin	RE-I	$C_{49}H_{78}S$	699.223	4
	RE-II	$C_{18}H_{10}S_2$	290.398	11
	RE-III	$C_{36}H_{57}N$	503.859	4
	RE-IV	$C_{29}H_{50}O$	414.718	1
	RE-V	$C_{40}H_{61}N$	555.935	3

curing agent, and asphalt, including four different models: three models of TOA modified with three different PEGs (EAP-200, EAP-400, and EAP-800) and a model of TOA for comparison (EA). Furthermore, the mass ratio of the curing agent to AC 70 asphalt was 1∶1. Periodic boundary conditions were selected. First, the molecular models of the epoxy resin and curing agent were added to 70# asphalt. To prevent molecular overlap and ensure reasonable configurations, the density of the initial model was set to 0. 5 g/cm³. The initial temperature of the model was set to 393 K, which was the curing temperature of the epoxy asphalt used in this study, to facilitate the simulation of subsequent crosslinking reactions. Then, the model was energy minimized using the Forcite module to achieve an optimal geometric configuration. Subsequently, to eliminate the stress generated during the modeling process and compress the model volume to make its density consistent with actual conditions, molecular dynamic simulations were performed on the optimized model in the NVT and NPT ensembles. COMPASS II can accurately simulate the physical and chemical properties of polymer materials as well as the interactions among molecules. Thus, it was selected as the molecular dynamics simulation force field. The temperature was set to 393 K, and the pressure was set to 1 atm in the NPT ensemble because this study was conducted at standard atmospheric pressure. The time step was set to 1 fs, and the total duration of the simulation was 400 ps (evenly divided into 200 ps in the NVT and NPT ensembles). Further, the Andersen and Berendsen methods were used as the temperature and pressure control methods in the simulation, respectively. Finally, epoxy asphalt bulks were obtained.

1. 3   Crosslinking procedure

According to the curing reaction mechanism (Fig. 2), an automatic crosslinking reaction program script between the epoxy resin and curing agent was written. Key parameters such as the minimum and maximum crosslinking radii were determined to be 0. 40 and 1. 55 nm, respectively, at increments of 0. 05 nm. Furthermore, the process involved five iterations per radius, which aimed for a target crosslinking degree of 90% at a controlled temperature of 393 K. Then, structure optimization of the crosslinked model was achieved by performing energy minimization using the Forcite module, which ensured an optimal geometric configuration. Subsequently, molecular dynamic simulations were performed on the optimized model in the NVT and NPT ensembles to eliminate the stress generated during the modeling process and to adjust the model volume, thus ensuring that its density was aligned with actual conditions. COMPASS II was used as the molecular dynamics simulation force field. Finally, the crosslinked model underwent annealing treatment, which resulted in the final crosslinked structure model of epoxy asphalt. Fig. 4 shows the amorphous and crosslinked molecular models of the EAP-200 epoxy asphalt. As the crosslinking reaction continued, the molecular structure gradually became closer, forming a 3D network structure.

(a)

(b)

Fig. 4 Molecular model of EAP-200 epoxy asphalt. (a) Amorphous model; (b) Crosslinked model

2 Tests, Results, and Discussion

2.1 Model validation and thermodynamic property analysis

Glass transition temperature is a thermodynamic property of a material and indicates the temperature at which a polymer changes from a glassy to a rubbery state. At the glass transition temperature, the material changes from a solid state to a soft elastomer, which leads to changes in its physical properties, including its specific volume, thermal properties, and mechanical characteristics. The glass transition temperature of epoxy asphalt is determined by analyzing the temperature-volume or temperature-density data obtained from MS. In the present study, molecular dynamics simulations were performed at different temperatures using the NVT and NPT ensembles to obtain the density of different epoxy asphalt materials at the corresponding temperatures. Fig. 5 shows the densities associated with various temperatures, along with the fitting curves of these models. The glass transition temperature of epoxy asphalt can be determined from the density-temperature data using segmented regression, which achieved an R^2 value of greater than 0.999 7 and a p-value of less than 0.000 1. The calculation results of the glass transition temperature are listed in Table 2.
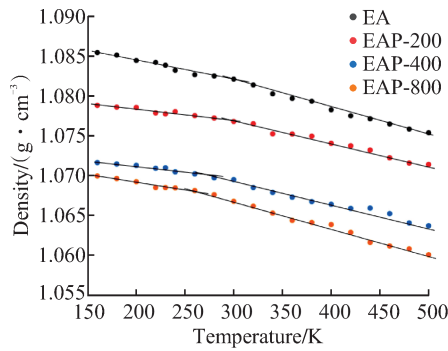

Fig. 5 Density-temperature fitting curve of the different epoxy asphalt samples

Table 2 Glass transition temperature of epoxy asphalt   K

Crosslinked system	Simulation results	Experimental results[15]
EA	304.96	291.15
EAP-200	294.03	278.25
EAP-400	275.15	262.75
EAP-800	262.97	247.35

Previous studies have shown that the dynamic thermodynamic properties of epoxy asphalt and PEG-modified epoxy asphalt were tested using dynamic mechanical analysis. Through analysis of the storage modulus curves, the experimental glass transition temperatures of various epoxy asphalt can be obtained, which are also listed in Table 2. It indicates that the change pattern of the glass transition temperature of epoxy asphalt calcu-

lated using MS was consistent with that of the experimental results, which indicated that the molecular models could be used for evaluating the properties of epoxy asphalt. However, the glass transition temperature calculated by MS was higher than that of the experimental result. This phenomenon occurred because the computational cooling rates were orders of magnitude faster than the experimental cooling rates. Therefore, when sampled on such short time scales, all-atom systems appeared glassy, whereas they were actually in a rubbery state.

The glass transition temperature of epoxy asphalt without PEG chain modification was higher than that of the epoxy asphalt modified with PEG chain, which indicated that PEG modification reduced the glass transition temperature of the epoxy asphalt, making it softer at low temperatures. The length of the PEG chain increased the flexibility of the polymer chain, thereby enhancing the segmental motion of the polymer. As the PEG chain increased, the glass transition temperature of epoxy asphalt gradually decreased, which indicated that longer PEG chain segments enable the material to maintain good flexibility at lower temperatures.

2.2 Mechanical property analysis

In this study, the mechanical properties of epoxy asphalt were calculated using the constant strain method in which a 0.02 small strain was applied. Epoxy asphalt can be regarded as an isotropic material. Its stiffness, shear deformation resistance, and compression resistance can be characterized by Young's modulus (E), shear modulus (G), and bulk modulus (K)[16].

$$E = \mu\left(\frac{3\lambda + 2\mu}{\lambda + \mu}\right) \qquad (1)$$

$$K = \lambda + \frac{2}{3\mu} \qquad (2)$$

$$G = \mu \qquad (3)$$

where λ and μ are the Lamé coefficients.

Table 3 lists the calculated mechanical properties of epoxy asphalt. The toughness of epoxy asphalt can be accessed using the ratio of bulk modulus to shear modulus (K/G). The higher the K/G value, the tougher the material[17].

Table 3 Modulus of different epoxy asphalt materials

Crosslinked system	E/GPa	G/GPa	K/GPa	K/G
EA	4.831	3.333	1.890	1.763
EAP-200	4.512	3.276	1.761	1.860
EAP-400	4.087	3.081	1.425	2.162
EAP-800	3.484	2.877	1.150	2.502

As the PEG chain length increased, the Young's modulus gradually decreased, indicating that the stiffness of the material gradually decreased. The introduc-

tion of PEG led to a reduction in the rigidity of the epoxy asphalt. The shear modulus gradually decreased as the PEG chain length increased, indicating that the resistance of the material to the shear stress became weaker. The bulk modulus also decreased with the increase in the PEG chain length, indicating that the material resistance to compression weakened. The changing trend of K/G was basically consistent with the glass transition temperature. As the PEG chain length increased, K/G gradually increased, indicating that the toughness of the material gradually increased. The PEG-modified epoxy asphalt may show better crack resistance and deformation adaptability in certain applications. By adjusting the PEG chain length, the mechanical properties of epoxy asphalt can be adjusted, resulting in different performance advantages in different applications.

2.3 Toughening mechanism

Mean square displacement (MSD) and free volume fraction can be used to explain the toughening mechanism. MSD reflects the changes in polymer chain mobility after PEG introduction, whereas the free volume fraction indicates the effect of PEG on the microstructure of epoxy asphalt.

2.3.1 Fractional free volume analysis

According to the free volume theory, the total volume of a liquid or solid material consists of the occupied volume (V_0) and free volume (V_f)[18]. Analysis of the free volume of epoxy asphalt from a molecular perspective can enhance understanding of its molecular packing and spatial state. The free volume diagram of EAP-200 is shown in Fig. 6. Because the total volume of different epoxy asphalt systems differs, a direct comparison of the free volumes among them is usually not feasible. In the present study, the fractional free volume (FFV) of different epoxy asphalt materials at 298 K is expressed as

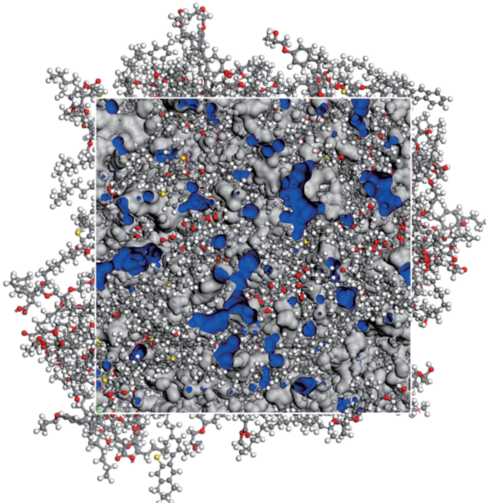$$F = \frac{V_f}{V_0 + V_f} \times 100\% \tag{4}$$

Fig. 6 Free volume diagram of EAP-200

Table 4 lists the FFV and density of the different epoxy asphalt samples. FFV represents the proportion of free volume inside the epoxy asphalt. The larger the FFV, the more the free volume of the epoxy asphalt and the higher the mobility of the molecular chain. Density represents the mass density of the epoxy asphalt. The higher the density, the denser the material.

Table 4 FFV and density of different epoxy asphalt samples

Property	EA	EAP-200	EAP-400	EAP-800
FFV/%	16.54	17.03	18.69	19.86
Density/(g·cm^{-3})	1.082	1.077	1.070	1.067

As the PEG chain length increased, FFV gradually increased, indicating that the free volume of epoxy asphalt increased because of the introduction of PEG. A longer PEG molecular chain resulted in a looser internal structure of the material and increased FFV. Further, the density of the epoxy asphalt gradually decreased with the increase in the PEG chain length, indicating that the material became looser and the structure became less dense. The introduction of PEG increased the spacing between the molecular chains, thereby reducing the density of the material. The changes in FFV and density indicated that the internal structure of the PEG-modified epoxy asphalt became looser, the molecular chain mobility increased, and the material density decreased. These changes helped enhance the flexibility of the epoxy asphalt; however, it also slightly affected its mechanical strength.

2.3.2 Mean square displacement analysis

MSD can characterize the ability of molecules to move in the model. During the particle diffusion process, MSD shows a linear relationship with time t, and its slope is represented by diffusion coefficient D. The calculations of MSD and diffusion coefficient D can be expressed as

$$M(t) = \langle |r_i(t) - r_i(0)|^2 \rangle \tag{5}$$

$$D = \frac{1}{6} \frac{\mathrm{d}\langle r_i(t)| - r_i(0)|^2 \rangle}{\mathrm{d}t} \tag{6}$$

where $r_i(t)$ and $r_i(0)$ are the position and initial position of the i-th atom at instant t, respectively. This study calculated the MSD of epoxy resin in the epoxy asphalt and compared the diffusion coefficients between the different epoxy asphalt samples.

Fig. 7 and Table 5 show the MSD results and diffusion coefficients of the epoxy asphalt, respectively. The larger the MSD and diffusion coefficient values, the stronger the molecule mobility.

The MSD value of epoxy resin in the different epoxy asphalt materials gradually increased over time, indicating that molecules were constantly moving and diffusing. The MSD value of the PEG-modified epoxy asphalt gradually increased with the increase in the PEG chain
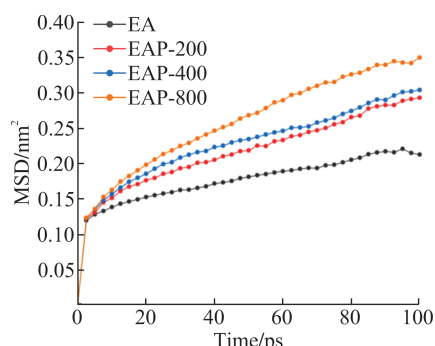
Fig. 7 MSD of epoxy resin in the different epoxy asphalt samples

Table 5 Diffusion coefficient of epoxy resin in the different epoxy asphalt samples

Sample	EA	EAP-200	EAP-400	EAP-800
Diffusion coefficient/10^{-3}	1.883	2.517	2.633	3.417

length, the diffusion coefficient also gradually became larger, and the activity of the epoxy resin molecules significantly increased. Among them, EAP-800 exhibited the highest MSD value and the largest diffusion coefficient, indicating that its epoxy resin molecules most actively moved and had the strongest diffusion ability. The introduction of PEG significantly affected the mobility of molecules in the material, which allowed it to exhibit better flexibility and plasticity in applications.

2. 4　Quantitative evaluation of epoxy asphalt cross-linked network

The elastic properties of epoxy asphalt are primarily influenced by a 3D network in which the crosslinking bonds are key factors in the formation of the 3D network. To evaluate the 3D network structure of epoxy asphalt, the shortest path from the crosslinked point to another crosslinked point can be calculated using the Dijkstra algorithm[19]. The contour length is measured in units of the number of linkages that must be traversed to travel across the network from a given crosslinking bond to another. The evaluation process can be described according to the following. The nodes and edges should first be defined, where the nodes represent the crosslinking bonds, and the edges represent the connections among them. The edge weights are based on the distance between the crosslinking bonds or other relevant parameters. A graph is constructed using an adjacency matrix. Subsequently, the shortest path for each crosslinking bond to all other crosslinking bonds can be calculated using the Dijkstra algorithm. The results are then recorded for further analysis. Because the sizes of each model are different, the crosslinking bond distance cumulative distribution curve is used to describe the changes in the crosslinking bond distance of each epoxy asphalt system.

Fig. 8 shows the distribution of the crosslinking bond distance in the different epoxy asphalt systems. The EA

curve is the steepest, indicating that the crosslinking bonds of EA are more concentrated and have a higher density. The curve of EAP-200 is slightly less steep than the EA curve, indicating a slightly more dispersed distribution and a slight density reduction in the crosslinking bonds when PEG-200 is added. The EAP-400 curve, with the addition of a longer PEG chain, becomes even flatter than the EAP-200 curve. The EAP-800 curve, which has the longest PEG chain, is the flattest. As the PEG chain length increases, the crosslinking density decreases and the molecular chain mobility of the epoxy asphalt increases. PEG modification can significantly change the crosslinking structure, thus enhancing material flexibility.
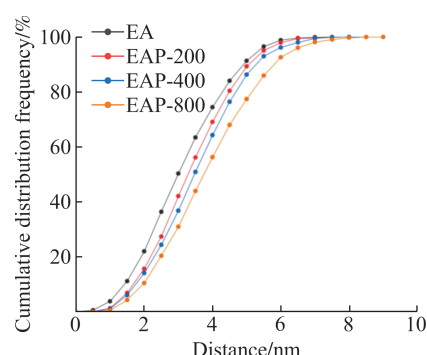

Fig. 8 Minimum crosslinking contour length distributions

3　Conclusions

（1）The change pattern of the glass transition temperature of epoxy asphalt calculated using MS exhibits good consistency with the experimental results.

（2）The thermodynamic properties of epoxy asphalt are significantly affected by PEG modification. The larger the chain length, the lower the glass transition temperature.

（3）The mechanical strength of epoxy asphalt weakens with the increase in the PEG chain length while the toughness increases.

（4）The activity space of epoxy asphalt increases with increasing PEG chain length, and the mobility of epoxy resin molecules in the epoxy asphalt increases, resulting in enhanced toughness.

（5）As the PEG chain length increases, the crosslinking bond paths lengthen, resulting in increased molecular mobility and enhanced toughness.

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聚乙二醇改性环氧沥青性能及增韧机理的分子尺度分析

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摘要：采用不同链长的聚乙二醇(PEG)对环氧沥青进行改性,基于分子模拟技术构建了 PEG 改性环氧沥青的分子模型。分析了 PEG 改性环氧沥青的热力学和机械性能,探讨了 PEG 改性环氧沥青的增韧机制,并开发了一种用于评价环氧沥青交联网络的算法。结果表明,引入 PEG 链可降低环氧沥青的玻璃化转变温度并增强其韧性,这归因于 PEG 链的延长可增加自由体积并改善环氧沥青中环氧树脂的流动性。采用基于 Dijkstra 算法提出的交联网络定量评价方法,可以有效评估环氧沥青交联点的分布,有利于理解 PEG 改性环氧沥青的增韧机制。验证了采用分子模拟进行设计和筛选环氧沥青材料的可行性,并为分子水平上的环氧沥青增韧机理研究提供了指导。

关键词：分子模拟;交联环氧沥青;热力学性能;力学性能;增韧机理

中图分类号：U414