Understanding interaction and dynamics of water molecules in the epoxy via molecular dynamics simulation

Lik-ho Tam, Denvid Lau and Chao Wu

School of Transportation Science and Engineering, Beihang University, Beijing, People’s Republic of China; Department of Architecture and Civil Engineering, City University of Hong Kong, Hong Kong, People’s Republic of China; Department of Civil and Natural Resources Engineering, University of Canterbury, Christchurch, New Zealand

ABSTRACT

The robust structural integrity of the epoxy plays an important role in ensuring the long-term service life of its applications, which is affected by the absorbed moisture. In order to understand the mechanism of the moisture effect, the knowledge of the interaction and dynamics of the water molecules inside the epoxy is of great interest. Molecular dynamics simulation is used in this work to investigate the structure and bonding behaviour of the water molecules in the highly cross-linked epoxy network. When the moisture concentration is low, the water molecules are well dispersed in the cross-linked structure and located in the vicinity of the epoxy functional groups, which predominantly form the hydrogen bond (H-bond) with the epoxy network, resulting in the low water mobility in the epoxy. At the high concentration, the water favourably forms the large cluster due to the predominant water–water H-bond interaction, and the water molecules diffuse primarily inside the cluster, which leads to the high water mobility and the accelerated H-bond dynamics. The variation of the bonding behaviour and dynamics of the water molecules reported here could be exploited to understand the material change and predict the long-term performance of the epoxy-based products during the intended service life.

1. Introduction

The epoxy material consists of a three-dimensional covalent network resulted from the cross-linking reaction at the molecular scale. Generally, the highly cross-linked epoxy material possesses good mechanical properties, which are important to ensure the robust structural integrity of the epoxy-based products. In recent years, the epoxy material has been frequently used in a wide range of the engineering applications at different length scales, from the microscale thin films in the microelectromechanical systems (MEMS), to the macroscale epoxy-based composite in the aerospace, automotive industries, and the civil infrastructures [1–4]. Due to the existence of the functional groups and the free volume in the cross-linked structure, the moisture can diffuse into the epoxy material [5]. Experimental methods have been used to investigate the diffusion of the water into the epoxy, the interaction between the cross-linked epoxy network and the absorbed water, and the moisture effect on the properties of the epoxy material [5–14]. Specifically, the absorbed water molecules interact with the epoxy cross-linked network mainly through the hydrogen bond (H-bond) interaction with the functional groups, which affect the structure and properties of the epoxy, such as the depression of glass transition temperature [6,8]. Meanwhile, our recent investigation of the cross-linked epoxy structure has shown that its Young’s modulus exhibits an initial increase after the two-week water bath conditioning, which decreases after the eight-week conditioning [14]. Such antiplasticisation phenomenon at the low moisture concentration has also been observed from other epoxy materials experimentally [10,11,13]. Furthermore, as the epoxy becomes less stiff over time due to the water sorption, it is anticipated that it could adversely affect the durability of the epoxy-based engineering applications under the moisture ingress. The properties of the epoxy material show a strong dependence on the moisture concentration in the system, and the knowledge of the structure and bonding behaviour of the water molecules in the epoxy structure is the key to understand the moisture effect.

Molecular dynamics (MD) simulation has been demonstrated as a versatile and fundamental tool to model the molecular structure of the epoxy material, investigate the atomistic interaction between the epoxy and water molecules, and predict the epoxy properties under the moisture effect [15–28]. Simulation studies have shown that the cluster formation of the water molecules becomes obvious with the increasing moisture concentration in the epoxy cross-linked network [25,28]. Meanwhile, it is found that the H-bond interaction varies with the moisture concentration in the epoxy system [15,25,26]. Specifically, a simulation study of a cured epoxy-amine structure has revealed that the three functional groups in the epoxy backbone (i.e. the hydroxyl, ether, and tertiary amine groups) are involved in the H-bond interaction with the water molecules, and when the moisture concentration increases, the added water molecules break up some of the existing H-bonds and forms the new ones with both the epoxy functional groups and other water molecules [15]. Moreover, the mobility of the water molecules is also affected by the moisture concentration in the systems,
where the diffusion of the water molecules generally increases with the increasing moisture concentration [19,20,25,26]. Although these simulation studies have provided useful information about the structure and properties of the water molecules confined in the epoxy material, it is still unclear about the local H-bond characteristics of individual water molecule and cluster in the epoxy structure, and the relationship with the dynamics of the water molecules, including the lifetime of the H-bond at various moisture concentrations. Such knowledge, in turn, can be used to understand the change in the structure and properties of the epoxy material during the intended service life.

This paper aims to investigate the local structure and H-bonding characteristics of the water molecules, and to study the water dynamics in the epoxy cross-linked networks at various moisture concentrations by using MD simulations. By utilising a computational cross-linking algorithm, the epoxy model with a high cross-linking density is constructed, which is solvated with various amounts of the water molecules. The local structure and H-bond network of the water molecules in the solvated structures are examined at the equilibrium local structure and H-bond network of the water molecules is solvated with various amounts of the water molecules. The model with a high cross-linking density is constructed, which is solvated with various amounts of the water molecules. The local structure and H-bond network of the water molecules in the solvated structures are examined at the equilibrium state, which are linked with the dynamics of the water molecules to understand the mechanism of the moisture effect. This study provides guidance towards exploring the interaction and dynamics of the water molecules in the cross-linked epoxy material, which is important for predicting the material durability during the long-term service life, and for improving the moisture barrier property of the epoxy-based products.

2. Model and simulation

In this investigation, the cross-linking process of the epoxy material is achieved computationally in the Materials Studio software [29], and the structural equilibration of the cross-linked network is carried out by using the open source code LAMMPS [30]. The molecular interactions are characterised by the consistent valence force field (CVFF) [31,32], and its applicability in investigating the epoxy material is validated in recent studies [14,33,34]. The water molecule in this study employs the TIP3P model [35]. During the equilibration process, the water molecule is simulated by adopting the SHAKE algorithm to keep the two bonds and the angle constant [36]. The van der Waals (vdW) and the short-range Coulombic force are measured with a truncated distance of 10 Å, while the long-range Coulombic force is measured by using the particle-particle particle-mesh (PPPM) solver [37]. The atom partial charges are estimated through the bond increment technique [38]. The integration of the equation of motion is achieved by adopting the velocity-Verlet integrator and a time step of 1 fs is used.

In this study, the epoxy model is constructed by the cross-linking process between the epoxy monomers at the molecular level. The chemical structure of the epoxy monomer is shown in Figure 1, which contains eight epoxide groups. During the model construction, the uncross-linked epoxy structure is firstly constructed, where a total of forty epoxy monomer molecules are placed in a three-dimensional periodic simulation cell. According to the commercially available data, the initial density is set to be 1.07 g cm$^{-3}$. The monomer quantity is determined by comparing the properties of the two epoxy models cross-linked from forty and eighty monomers, which are in good agreement, suggesting that a small-scale model is capable of characterising the structure and properties of the cross-linked epoxy [34]. Subsequently, the uncross-linked epoxy model is subjected to an initial relaxation process at the temperature of 300 and 368 K, respectively. The elevated temperature of 368 K is normally adopted for the epoxy cross-linking process in the experiment. At each temperature, the epoxy model is equilibrated in the canonical (NVT) ensemble for 10 ps, and then in the isothermal-isobaric (NPT) ensemble at the pressure of 1 atm for 10 ps. The temperature and the pressure are controlled under the Nosé thermostat [39,40], and Andersen barostat [41], respectively.

After the initial structural equilibration, the epoxy model is cross-linked by adopting the dynamic cross-linking algorithm [34]. Detailed steps involved in this algorithm are described in our previous studies [14,34,42,43]. In this algorithm, the cross-linking reaction is simulated in a step-wise manner by using the distance-based approach, which allows the epoxy model to be rid of the severe structural distortion and possess the high cross-linking density. After that, the epoxy structure is subjected to the equilibration process at the temperature changing from 368, 334, to 300 K, respectively. The equilibration process is similar to the initial relaxation as described previously. During the reaction process, the epoxy cross-linking density increases gradually with the reaction radius, and the final cross-linking density of the epoxy model reaches 82%, which is consistent with the synthesised polymer materials through different experimental approaches [44,45]. After the cross-linking process, the epoxy cross-linked network is further relaxed by using the relaxation scheme as validated previously [34]. Specifically, the epoxy model is relaxed in seven equilibration cycles at the temperature of 300 K in both the NVT and NPT ensembles. During the NPT relaxation, the applied pressure in the first three cycles increases steadily from 1 to 50,000 atm. Under the large pressure applied in these processes, the cross-linked structure is compressed efficiently. In the subsequent four equilibration cycles, the applied pressure reduces gradually to the atmospheric pressure, and the epoxy model is decompressed efficiently when the applied pressure decreases.

Figure 1. The chemical structure of the epoxy monomer.
gradually. Under the equilibration cycles comprising these pressure controls, the polymer material can possess the density with improved accuracy [34,46,47]. Finally, the cross-linked network is relaxed at 300 K and 1 atm for 8 ns. During the equilibration run, the root-mean-square displacement (RMSD) of the atoms is examined, which reaches a relatively constant level before the equilibration is finished, implying that the equilibrium state is achieved. The Nosé–Hoover thermostat and barostat are used for the temperature and pressure control, respectively [48].

To study the structure and properties of the water molecules in the epoxy material, the equilibrated epoxy structure is solvated with various amounts of the water molecules to mimic the different moisture absorption states in the real case. It is reported that the maximum moisture absorption is under 4.0 wt% of different epoxy materials [6,8,27,49]. In this work, the amount of the water molecules added into the structure is 1.0 and 4.0 wt% of the molar mass of the cross-linked network, which is considered as the initial and equilibrium absorption condition, respectively. The added water molecules are well dispersed in the epoxy cross-linked structure, as shown in Figure 2.

After the model construction, the cross-linked structures with different moisture concentrations are subjected to the equilibration process. Specifically, the models are relaxed in the NPT ensemble at 300 K and 1 atm for 20 ns. By monitoring the RMSD of the epoxy atoms during the equilibration run, the fully equilibrium state is confirmed.

3. Results and discussion

The results obtained from the MD simulations are presented here, including the discussions about the structure, properties, and dynamics of the water molecules in the cross-linked epoxy structure at various moisture concentrations.

3.1. Bonding behaviour of the water molecules

After the equilibration process, the equilibrated conformations of the epoxy structures with various moisture concentrations are shown in Figure 3. At the low moisture concentration, i.e. 1.0 wt%, the water molecules are still uniformly dispersed in the cross-linked structure. When the moisture concentration is high, the water molecules in the structure form the clusters with the large size and quantity. The different structural conformations of the water molecules at various moisture concentrations agree very well with the recent experiment study on

Figure 2. (Colour online) The epoxy structures with the addition of (a) 0.0, (b) 1.0, and (c) 4.0 wt% of the water molecules.
the SU-8 epoxy photoresist by using the optical microscope [14]. For the samples in the dry condition, it is observed that the SU-8 is highly transparent, while for the samples after the two-week moisture conditioning, the microscope result shows that there are some black particles in the SU-8 structure. The simulation results here signify the different structure of the water molecules in the epoxy networks, which could be related to the different bonding behaviours and dynamics of the water molecules.

In order to understand the bonding behaviour of the water molecules, the location of the water molecules in the epoxy structure is analysed first, which is determined by computing the free volume change of the cross-linked structure with the addition of the water molecules. Specifically, the Connolly surface algorithm is used [24,50]. In this algorithm, a probe sphere with a radius of 1 Å is rolled over the surface of the cross-linked network to draw a smooth, continuous, and three-dimensional contour surrounding the epoxy structure, and the volume not covered by the contour is regarded as the free volume, which can be computed analytically. During the 20 ns NPT relaxation run, the fractional free volume of the epoxy networks is recorded every 5 ps. The data from the last 100 ps relaxation run are averaged and shown in Figure 4, with respect to the moisture concentration. When the moisture concentration increases, the fractional free volume of the epoxy decreases, which indicates that the added water molecules appear to be located in the free volume available in the epoxy cross-linked network. Especially, at the high moisture concentration, the water molecules form the cluster with the large size, which fills the available free volume in the structure and leads to the decrease of the fractional free volume.

Apart from the favourable distribution in the free volume, the location of the water molecules is affected by the functional groups in the epoxy structure. In the backbone of the epoxy structure, there are two important potential hydrogen bonding sites, including the hydroxyl groups and ether groups, which are highly electrophilic in nature and tend to interact with the water molecules by forming the H-bonds. The radial distribution function (RDF) quantifies the normalised probability of finding a particle at a distance $r$ from another particle, which is used to understand the packing of the water molecules around the epoxy functional groups. The RDF between the oxygen atoms in the water molecules and the oxygen atoms in the epoxy functional groups is measured as shown in Figure 5. It is seen that the RDFs for the hydroxyl–water and ether–water interactions show similar peaks at two distances. The sharp peak at the shorter distance is an indication of the formation of the H-bond between the functional groups and the water molecules, whereas the second peak at the distance of around 5.0 Å indicates the distance between the neighbouring hydroxyl groups and the water molecules for the hydroxyl–water interactions, and for the ether–water interactions, it is associated with the ether groups in the newly created cross-links and the symmetry of ether groups in the epoxy network. Meanwhile, the peak intensity of the hydroxyl–water RDFs is comparatively higher at the shorter distance, which implies that the water molecules pack favourably around the hydroxyl groups rather than the ether groups. The reason could be due to the fact that the hydroxyl group offers two potential H-bond sites as both the oxygen and hydrogen of the functional groups can form an H-bond with the water molecule, while the ether groups only offer one potential H-bond site. Furthermore, it is observed that the peak intensity is affected by the moisture concentration, which drops when the moisture concentration increases.
concentration is high. It is owing to the fact that in the epoxy network, there is a constant number of the hydroxyl groups and the ether groups, and the portion of the water molecules involved in the H-bonds interaction with the cross-linked structure decreases when the moisture absorption increases, which results in the decrease in the intensity of the peak at the high concentration. From these observations, it is demonstrated that the water molecules tend to diffuse to the free volume available in the epoxy network, and also in the vicinity of the epoxy functional groups, which affects the intra-molecular interactions of the epoxy network.

To characterise the molecular interaction between the water molecules and the epoxy structure, the H-bond network in the system is of interest. Firstly, the H-bond quantity formed among the epoxy functional groups, between the epoxy and the water molecules, as well as among the water molecules is examined. The H-bond is formed when the two geometric criteria are satisfied: the distance between the donor consisting of the hydrogen atom and the acceptor is under 3.5 Å and the angle formed by the donor-hydrogen-acceptor is above 130° [51]. The value of the H-bond cutoff distance corresponds to the first minimum location in the RDFs as shown in Figure 5. To determine the water–epoxy H-bond, it considers all of the potential H-bond interaction sites in the epoxy model, including both the hydrogen and oxygen atoms in the hydroxyl groups and the oxygen atoms in the ether groups. The recorded data from the last 0.5 ns equilibration run are shown in Figure 6 (a), with respect to the moisture concentration. It is observed that the H-bond quantity between different constituents keeps at a relatively constant level over time, which indicates that the H-bond formation of the water molecules in the epoxy structure reaches the equilibrium state. Particularly, with various moisture concentrations, there has a relatively small effect on the H-bond formation among the epoxy functional groups, which corresponds to the previous observation that the water molecules tend to be located in the free volume available in the structure, and indicates that the existing epoxy–epoxy molecular interactions are maintained to a certain extent in the wet condition. Based on the recorded H-bond quantity, the fraction of each type of the H-bond is calculated as shown in Figure 6(b). Specifically, the intensity of the epoxy–water H-bond is more pronounced than that of the water–water H-bond at the low moisture concentration, while the water–water H-bond appears to dominate at the high concentration. The variation of the H-bond fraction demonstrates the different bonding behaviours of the water molecules in the epoxy networks with various moisture concentrations.

After characterising the global bonding behaviour between the water and epoxy, the local H-bond characteristics of the water molecules are examined by focusing on the probabilities of the water–epoxy and water–water H-bond formation for a randomly selected water molecule. The calculated H-bond probability distribution at different moisture concentrations is shown in Figure 7. Independently, the H-bonds are defined according to a different cutoff angle, i.e. the donor-hydrogen-acceptor angle is above 140°, and the calculated H-bond probability distribution shows no obvious difference from the reported result. As seen from the H-bond distribution, there are a portion of the water molecules having no H-bond interaction with the epoxy network and other water molecules, which exist as the single water molecules. The interactions of these single water molecules and the epoxy structure are minimal, which can only weakly affect the intra-molecular interaction of the epoxy structure. When the moisture concentration in the system is low, i.e. 1.0 wt% in this study, apart from the single water molecules, a large number of the absorbed water molecules forming the water-epoxy H-bonds,
but almost forming no H-bond among the water molecules. These observations are consistent with the recent simulation studies of the polyacrylate polymer and the epoxy nanocomposite, where the water molecules predominantly form H-bonds with the polymer matrix when the moisture concentration is low [42,52]. With the high moisture absorption, more water molecules are involved in the H-bond interaction with other water molecules. The water molecules interacting with other water molecules can form the aggregated water clusters, as shown in Figure 3. Though usually they are not big enough to resemble bulk water properties, these water clusters filled in the available space of the structure can influence the intra-molecular interactions of the epoxy structure.

From the previous simulation results, it is observed that when the moisture concentration increases, the water molecules preferably form a large number of the water–water H-bonds rather than forming the H-bonds with the epoxy, which leads to the formation of the water clusters. Information about the structure of the water clusters in the system can be obtained by quantifying the probability of the water cluster size. The water molecules belong to the same cluster when their oxygen atoms are within a cutoff distance value of 3.5 Å and are also less than a cutoff donor-hydrogen-acceptor angle of 50°, as similar to the geometric criteria of the H-bond formation stated previously. The cluster size probability distribution for the epoxy systems with various moisture concentrations is shown in Figure 8. It is noted that the ordinate implies the probability of belonging to a water cluster of a given size for a randomly selected water molecule. At the low moisture concentration of 1.0 wt%, only about 34% of the water molecules exist in the form of pairs to form the small cluster, while the majority exists as the individual molecule in the epoxy system. At the high moisture concentration, the clustering behaviours of the water molecules are obvious, where more water molecules are participated in forming the large cluster in the epoxy, including the single, very large cluster containing 27 water molecules. For the investigated small-scale epoxy model, there is limited free volume in the structure, and hence other clusters are formed with a smaller size, which contain water molecules up to 16. Therefore, the cluster with water molecules in the range of 17 to 26 is not formed in the constructed model, leading to the zero probability in this range as shown in Figure 8. It is inferred that for the epoxy model with a larger size, it possesses increased structural free volume, which can promote the formation of water cluster with the more consistent size. However, the observation of increased water cluster size with increasing moisture concentration in the system could be relatively the same, due to the electrophilic nature of water molecules. Furthermore, the observed trend is in a good agreement with the observation reported for the water clustering behaviour in different polymer and composite materials [25,42,52].

Further insight into the interaction of the water molecules in the system can be obtained by focusing on the probabilities of forming the water–epoxy H-bond for a given water cluster. The formation of the H-bond is examined based on the two geometric criteria of the donor-acceptor distance and the donor-hydrogen-acceptor angle as stated previously. The calculated H-bond probability distribution at different moisture concentrations is shown in Figure 9. Some of these water clusters do not form the H-bonds with the epoxy network, analogous to the single water molecules, which can be considered as the single water clusters. At the same time, the rest of the water clusters can form the H-bonds with the epoxy network, including the Group I water cluster forming one H-bond with the epoxy system, and the Group II water cluster with more than one water–epoxy H-bond. Among the various moisture additions, the probability of being Group II water cluster is largest, and the bridging effect of these clusters can effectively affect the intra-molecular interactions of the epoxy structure. Particularly, these clusters connect two or more functional groups in the epoxy network through the water–epoxy

![Figure 7](https://example.com/figure7.png)

*Figure 7.* (Colour online) The H-bond probability distribution for a given water molecule in the epoxy structures as a function of the moisture concentration: (a) 1.0 wt%; (b) 4.0 wt%. The E–W and W–W H-bonds denote the epoxy–water and water–water H-bonds, respectively.

![Figure 8](https://example.com/figure8.png)

*Figure 8.* (Colour online) The cluster size distribution of the water molecules in the epoxy structures as a function of the moisture concentration.
H-bonds, which leads to the creation of the secondary cross-links, and may result in the stiffening of the epoxy structure at the low moisture concentration [10,11,13,14].

3.2. Dynamics of the water molecules

After characterising the bonding behaviour between the water molecules and epoxy, the dynamics of the water molecules are examined. As the water molecules diffuse inside the epoxy structure, the bonding network in the system is continuously broken and reformed over time, including the H-bond network as examined previously. To quantify the dynamics of the H-bond, the time autocorrelation function (ACF) is calculated according to Equation (1),

\[ C(t) = \frac{\langle b(0) \cdot b(t) \rangle}{\langle b^2(t) \rangle} \tag{1} \]

where \( b(t) \) is a binary operator which takes a value of one if a particular tagged pair (i.e. hydrogen bonded at time \( t = 0 \)) of molecules is hydrogen bonded at time \( t \), and zero otherwise; \( \langle \cdot \rangle \) in this equation denotes the ensemble average over all the H-bond pairs in the system. In the calculation, \( b(t) \) takes a value of one only if the same tagged pairs remain hydrogen bonded continuously from time \( t = 0 \) to time \( t \), and the motion of the water molecule that can break an existing H-bond can lead to a decay of the time ACF. The calculated time ACF of the water–water H-bond for the epoxy systems with various moisture concentrations is shown in Figure 10. The correlation function decays rapidly for the system at the high moisture concentration, whereas the decay is slower for the epoxy structure with a lower moisture concentration. To quantify this phenomenon, the calculated ACFs are fitted by the Kohlrausch-Williams-Watts functional form \( C(t) = \exp[-(t/\tau)^\beta] \), where \( \tau \) and \( \beta \) denote the relaxation time and stretching exponent, respectively [53]. The relaxation time \( \tau \) is 11.5 and 8.4 ps for the epoxy with the moisture concentration of 1.0 and 4.0 wt %, respectively. This observation suggests that with the presence of a large number of water molecules at the high moisture concentration, the water molecules break the existing water–water H-bond and form the new ones with other water molecules more frequently, which accelerates the H-bond dynamics in the epoxy structure.

Apart from the H-bond dynamics, the mobility of the water molecules is another important parameter to characterise. During the equilibration, the MSD of the water molecules is monitored in the systems with various amounts of water molecules, which are plotted as a function of the simulation time, as shown in Figure 11. Accordingly, the MSD data are fitted by using the least square method. The slope of fitted curve in the system with 1.0 wt% moisture concentration is 0.37, which is smaller than that in the system with 4.0 wt% moisture concentration with a value of 0.47, demonstrating the difference in the mobility of the water molecules. The result can be explained by considering the effect of moisture concentration.
In this study, MD simulations are carried out to study the high moisture concentration, which allows the water molecules to travel a long distance without encountering the epoxy matrix, and thus, the water molecules diffuse primarily inside the cluster and subsequently show a high mobility. At the low moisture concentration, the water molecules primarily interact with the epoxy network and hence have a low mobility. By using the simulation approach at the molecular level, it is discovered that the bonding behaviour and dynamics of the water molecules are highly affected by the moisture concentration absorbed in the epoxy system. It is proved that under the environmental exposure, the material change of the epoxy is highly correlated with the absorbed moisture, as it is observed for the difference in the structure of water molecules and in the H-bond interaction with the epoxy networks observed from the three investigated conditions, i.e. the dry, initial, and equilibrium absorption condition. The MD simulation results reported in this study provide the direct observation of the interaction between the epoxy and water molecules, which are difficult to be characterised by the experimental approach as it lacks the suitable temporal and spatial resolution. In previous atomistic simulations, it is reported that the structure and properties of the epoxy material are significantly affected by the absorbed moisture, but the microscopic detail of the bonding characteristics of individual water molecule and cluster is not provided [15,25,26]. Furthermore, the relationship observed here between the bonding and dynamics of the water molecules is largely resulted from the fact that the highly dipolar water molecules possess the strong interactions with the functional groups and other water molecules. Therefore, it is believed that the results reported here are applicable to understanding the water behaviour in the epoxy-based systems involving the highly cross-linked structure.

4. Conclusions

In this study, MD simulations are carried out to study the mechanism of the moisture effect on the cross-linked epoxy material, with the focus on the interaction and dynamics of the water molecules inside the structure. Using the dynamic cross-linking algorithm, the epoxy network is modelled with a high cross-linking density consistent with the available data. With different amounts of the moisture concentration, the structure and bonding behaviour of the water molecules in the epoxy network are affected significantly. Due to the electrophilic nature of the functional groups in the epoxy, the added water molecule has the strong affinity for these functional groups and affects the H-bond dynamics and water mobility inside the epoxy structure. When there is a scarcity of the moisture in the epoxy structure, a majority of water molecules form the H-bond with the epoxy network, which results in the low H-bond dynamics and water mobility in the epoxy. As the moisture concentration increases, the water molecule forms a larger number of the water–water H-bonds, which results in the formation of the large clusters inside the structure, and leads to the accelerated H-bond dynamics and high water mobility. The observation of the bonding interaction and dynamics of the water molecules with various moisture concentrations that is elucidated here is of great use for analysing the results from the laboratory experiments, such as understanding the texture change of the epoxy photoresist examined after different durations in the moisture conditioning. Overall, the results reported here could be used to relate the microscopic information obtained at the nanoscale to the material behaviour at the macroscale, which are useful for predicting the moisture affected global performance of the epoxy-based products at multiple length scales.

Disclosure statement

No potential conflict of interest was reported by the authors.

Funding

This work was supported by the National Science foundation of China [grant number 51608020 and 51808020]; the Thousand Talents Plan (Young Professionals) in China; and the China Postdoctoral Science Foundation [grant number 2017M620015 and 2018T110029].

ORCID

Lik-ho Tam http://orcid.org/0000-0002-8592-1911
Denvid Lau http://orcid.org/0000-0003-3454-3938
Chao Wu http://orcid.org/0000-0001-8258-3227

References


Accelrys Software Inc. Materials Studio; 2009.


