EVA enhances the interfacial strength of EPS concrete: a molecular dynamics study

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ABSTRACT
Expanded polystyrene (EPS) concrete has high environmental and economic benefits. However, the difference in physical and chemical properties leads to a weak interface between EPS and concrete, which limits the use of EPS concrete. Based on the macro experiment of Ethylene Vinyl Acetate Copolymer (EVA) modified EPS concrete, two molecular dynamics interface models of EPS/C-S-H and EPS/EVA/C-S-H were constructed by molecular dynamics simulation, and their interface strengthening mechanism was discussed. The results of interfacial interaction analysis show that EVA increases the interfacial interaction energy and binding energy between EPS and C-S-H, and improves the adhesion between EPS and cement base. The results of radial distribution function analysis show that in the model with the modifier, there are not only Van der Waals forces and hydrogen bonds in the model without the modifier, but also strong interactions such as Ca – O and O – O. The results of mechanical property analysis show that the elastic modulus of EPS concrete interface model after adding modifier is improved, and its interface properties are improved. The molecular dynamics simulation carried out in this paper shows that EVA acts as a bridge between EPS and C-S-H and enhances its interfacial properties. This study can provide basic theoretical support for the application of EPS concrete and reference for the development of high-performance composite cement-based materials.

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1. Introduction

Expanded polystyrene (EPS) concrete is a kind of organic and inorganic composite light aggregate concrete, with EPS particles partially or wholly replacing the light aggregate in concrete, forming EPS concrete or EPS mortar. Compared with ordinary concrete, it has a smaller density, lighter weight, better thermal insulation performance, and sound insulation performance. It can significantly reduce building energy consumption and the weight of the structure. At the same time, it is also an ideal wall thermal insulation material. In addition, EPS concrete consumes a large amount of recyclable daily waste—EPS foam, which solves the problem of environmental pollution [1–4]. It is a kind of building material with high economic, social and environmental benefits, and has a broad application prospect in many fields, especially in the field of building structures and traffic roads.

However, in practical application, EPS is easy to separate from concrete due to the difference in physical and chemical properties between EPS and concrete, which leads to stratification between EPS and concrete (Figure 1a) [5]. In addition, this difference also

Figure 1. EPS concrete engineering defects. (a) Delamination, (b) force damage.
leads to the weak interface transition zone between EPS and concrete. In the case of compression failure and tensile failure (Figure 1b), the interface transition zone is effortless to form micro-cracks. These micro-cracks will be further aggravated in the loading process, resulting in the loss of mechanical strength and limiting its engineering application. Therefore, one of the keys to improving the strength of EPS concrete is to improve the interface bond strength between EPS particles and cement slurry. Zhao et al. [6] chemically modified the surface of EPS particles with the mass of ethylene-vinyl acetate (EVA) emulsion accounting for 0%, 5%, 10%, and 15% of the mass of cement, and found that the surface modification of EPS by EVA could increase the compatibility between EPS and inorganic matrix. To improve the microstructure of EPS lightweight aggregate concrete and make the cement hydration more efficient, the composition of hydration products can be optimized, so that the compressive strength and bending strength of EPS concrete can be improved. In terms of building materials, the polymer EVA is a common energy-saving and environmental protection modifier. It modified various composite building materials in flexibility, impact resistance, bonding strength, stability, and other aspects that have been greatly improved. To reveal the influence of the structure of polymers and modifiers on the morphology and interfacial interaction of composites, the structure, and properties of composites have been extensively studied. Li et al. [7] studied the effect of EVA emulsion on the interfacial strength of glass fiber reinforced magnesium oxide cement composites. Ru et al. [8] studied the effect of styrene-butadiene rubber (SBR) emulsion on the physical and mechanical properties of cement mortars based on SEM and IR analyses. The results show that the properties of the polymer-modified mortars are influenced by the polymer film, cement hydrates, and the combined structure between the organic and inorganic phases. Babu et al. [9] studied the performance of concrete containing fly ash EPS aggregate and compared it with the results of concrete containing OPC only as of the binder in literature.

Although there have been a lot of studies on this kind of topic, especially the studies of EVA modified EPS concrete are mostly focused on the experiment of macroscopic and microscopic mechanical properties, yet the mechanism of its nano-scale interface strengthening is still unknown. Researchers at home and abroad have found that molecular dynamics simulation (MD) can be used to study the interaction mechanism at the nanoscale. Zhang et al. [10] used MD to study the interaction between polymers with and without coupling agents and hydroxyapatite, compared and analyzed the confinement energies of the three planes, which made an important contribution to the research and development of artificial bones. Katti et al. [11] studied morphology, molecular interaction, and physical properties of organo-modified montmorillonite and polymer clay nanocomposites by the MD method. Yu et al. [12] used MD to study the improvement of chloride ion corrosion resistance of matrix by modifying rubber calcium silicate hydrate nanopores with silane. Kaynak et al. [13] reported that the carbon fiber which is processed by A174 significantly improved the mechanical properties of carbon fiber/epoxy resin composites. All in all, Molecular dynamics simulation (MD) is an effective way to study the interfacial interactions between inorganic fillers, polymer substrates, and modifiers or coupling agents [14–17]. Therefore, in this study, it is assumed that EVA could bridge EPS particles and cement slurry in EPS cement slurry composites, thus improving interface bonding and overall mechanical strength. The interaction energy, radial distribution function, and mechanical properties are calculated by the above molecular dynamics method. By exploring the enhancement mechanism of EVA on EPS/C-S-H at the molecular scale, the effects of EVA on the macroscopic properties and fine and microscopic structure of EPS concrete composite materials were verified (Figure 2).
provides the basic theoretical support for the use of EPS concrete and has the guiding significance for the future development of better quality EPS concrete.

2. Simulation methods

2.1. Model construction

2.1.1. EPS/C-S-H interface model

To reveal the mechanism of EVA enhancing EPS concrete interface, this study established two interface model systems through MD simulation and simulated them respectively under the same conditions. As one of the important parts of the research, concrete is a kind of composite material that can exert its mechanical properties only by cement bonding. Calcium silicate hydrate (C-S-H) is the most important binding phase in cement-based materials, accounting for 60%–70% of hydration products, which determines the mechanical properties and durability of cement-based materials [18]. In addition, the crystal structure of Tobermorite11Å was used as the starting model in this study (Figure 3d), which was successfully applied to the performance evolution of C-S-H in the study of the structure and dynamics of C-S-H gel [19–23]. XRD experiments of C-S-H show that the atomic structure of the smallest C-S-H gel unit is a layered crystal structure, similar to the atomic structure of the mineral tobermorite11 Å [24]. Therefore, it can be considered that the feasible method of establishing the C-S-H gel model depends on tobermorite11 Å crystal cells. The crystallographic parameters are as follows: (1) Crystal system: monoclinic. (2) Cell parameters: $\alpha = \beta = 90^\circ$, $\gamma = 123.49^\circ$, $a = 6.69$ Å, $b = 7.39$ Å, $c = 22.77$ Å. (3) Space point group: P2$_1$. Expanded it twice along X, triple along Y, and kept the Z direction unchanged to form a supercell. Besides, to establish the inter-facial phase between
tobermorite and EPS, a parallel C-S-H substrate with the size of $22.3\,\text{Å}/C\times22.2\,\text{Å}$ was obtained by shearing C-S-H along with the [0 0 1] direction (z-direction).

EPS is made of polystyrene particles foamed, and polystyrene particles mainly contain polystyrene, which is a polymer synthesized by styrene monomer through free radical intensified reaction. In this study, the literature [25] was used to calculate the solubility parameters of the polymer EPS optimal degree of polymerization is 60. Therefore, first, we used Build Polymers to construct a random EPS polymer chain (Figure 3b) containing 60 styrene monomers (Figure 3a) and containing 962 atoms (C:480 H:482). After that, an amorphous crystal cell (Figure 3c) with the same size as C-S-H a and b ($22.3\,\text{Å}/C\times22.2\,\text{Å}/C\times16.4\,\text{Å}$) and a density of $1.282\,\text{g/cm}^3$ were constructed by using Amorphous cells with the obtained polymer chain under the condition of 298 K and accuracy of Fine. After optimization, the optimal configuration with the lowest energy was selected as the initial input configuration. Secondly, build layers were used to set the XY plane of C-S-H in contact with the amorphous cell of EPS after optimization. Finally,
three-dimensional periodic boundary conditions were set and a vacuum layer of 40 Å was added so that the polymer could only interact with one side of the hydrated calcium silicate surface to ensure that there is no interaction with the periodic image of the computing unit. At the same time, the size of the system box along the vertical direction is large enough to fully observe the configuration change of the polymer on the C-S-H surface. The final cell parameters are about 22.3 Å × 22.2 Å × 91.6 Å and contain 1514 atoms (C:480; H:332; O:516; Si:108; Ca:78). The adsorption snapshots before and after simulation are shown in Figure 3(e) and 3(f), in which the EPS polymer is shown in yellow for a better display effect.

2.1.2. EPS/EVA/C-S-H interface model
Ethylene Vinyl Acetate Copolymer (EVA) is a thermoplastic resin composed of non-polar ethylene monomers and strongly polar vinyl acetate monomers. The higher the content of vinyl acetate, the stronger the bond performance, the greater the polarity, and its molecular formula is \((\text{C}_2\text{H}_4\times (\text{C}_4\text{H}_6\text{O}_2)\times y)\). Firstly, EVA random copolymer chain (Figure 4c) with monomer ratio of ethylene (CH2 = CH2) (Figure 4a) to vinyl acetate (Figure 4b) of 3:7 and polymerization degree of 10 was constructed by Build Polymers. Then, an amorphous battery was used to construct a two-dimensional amorphous hybrid model (Figure 4e) (the weight ratio of EPS to EVA was 2:1) at the specified temperature (289 K) and quality (fine), with a density of 1.03 g/m³ and a size of about \(\alpha = \beta = \gamma = 90^\circ\) and 22.3 Å × 22.2 Å × 47.3 Å, and the atomic number is 2210 (C: 888; H:1154; O:168). Finally, a two-layer model was established by using the optimized EPS/EVA amorphous hybrid model and C-S-H interface model, and a 40 Å vacuum layer was set, and its cell parameters are about 22.3 Å × 22.2 Å × 120 Å and contain 2,792 atoms (C:888; H:1202; O:516; Si:108; Ca:78).

![Figure 4.](image-url) (a) Ethylene monomer, (b)vinyl acetate monomer, (c) EVA chain, (d) EPS chain, (e) EPS/EVA amorphous mixed model, (f)/(g) EPS/EVA/C-S-H interface model and before/after simulation snapshots (Color legend: hydrogen H (white sphere and stick); calcium Ca (green sphere); oxygen O (red sphere and stick); silica Si (yellow sphere and stick); ethylene-vinyl acetate copolymer EVA (blue chain); polystyrene EPS (yellow chain)).
Si:108; Ca:78). The adsorption snapshots before and after simulation are shown in Figure 4(f) and 4(g). For better display effect, EPS is shown in yellow and EVA in blue.

2.2. Forcefields and simulation details

The proper selection of force field is a very important step in carrying out molecule simulation. It will lead to an accurate model for potential energy hypersurface in the moving of nuclei. COMPASS field is the first molecular force field to unify the field of organic and inorganic molecular systems, which can effectively predict the microstructure and dynamic properties of polymer materials. In addition, since it can capture most of the energy calculations and the potential energy of interactions between different atoms and molecules in silicic acid materials, and COMPASS has been proved to be in good agreement with its experimental data, the COMPASS field is perfectly suitable for the simulation of cement hydration products [24,26].

The simulation of this study was carried out at room temperature (298 K). Although the first 24 h of the cement hydration process is exothermic and generates a large amount of heat, the main content of this study is carried out under the load-bearing condition of the model. Thus, room temperature can be set to simulate the C-S-H/polymer interaction after the hydration reaction. The force field selected by optimization and annealing is unified as the COMPASS force field. In addition, the model molecule is large, so to make the system better overcome the barrier between the local minimum values on the potential energy surface, this paper first carries out structural optimization, which eliminates the local unreasonable structure generated in the process of model construction and ensures the model convergence. The lowest energy state model is selected for 20 cycles under the NVT ensemble. Each cycle is heated from 300 K to 800 K and then reduced to 300 K with a temperature gradient of 50 K, and the time of each annealing process is 200 ps. After that, under the condition of 298 K, the annealed model is carried out at a kinetic equilibrium of 300 ps. After the calculation, the model is stable as the temperature remains near 298 K and the energy tends to be stable [27]. The trajectory data of the last 100 ps is stored for subsequent dynamic analysis. More detailed simulation details are shown in Table 1.

3. Results and discussion

3.1. Interaction energy and binding energy

Interaction energy reflects the magnitude of the interaction between the inorganic phase and the organic phase [28]. The binding energy is an important criterion to evaluate the adhesion and miscibility between C-S-H and polymer [10,29,30], and their interactions are negative. The calculation formula of the interaction energy $E_{\text{inter}}$ is shown in Eqs. (1) and (2).

$$E_{\text{inter}1} = E_{\text{total}1} - (E_{\text{surface}} + E_{\text{polymer1}})$$  \hspace{1cm} (1)

$$E_{\text{inter}2} = E_{\text{total}2} - (E_{\text{surface}} + E_{\text{polymer2}})$$  \hspace{1cm} (2)

where $E_{\text{inter}1}$ is the interface interaction energy of EPS concrete without modifying agent, $E_{\text{inter}2}$ is the interface interaction energy of EPS concrete with modifier added, $E_{\text{surface}}$ and

|  | Nonbond Vdw, Coulomb | Simulation method | Ensemble | Temperature | Cutoff R | Initial velocities |
|---|---|---|---|---|---|---|
| Algorithm | Max. iteration | Quality | Total number of steps | Time step | Frame out |
| Smart | 20,000 | Fine | 500,000 | 1fs | Every 500 steps |

Table 1. Detailed simulation details.
$E_{\text{polymer}}$ are respectively the energy of crystal surface and EPS polymer chain, $E_{\text{total1}}$ is the total energy of the crystal surface and polymer with C-S-H, $E_{\text{polymer2}}$ is the total energy of an amorphous polymer mixed with EPS and EVA, $E_{\text{total2}}$ is the energy of a C-S-H surface and an amorphous polymer mixture.

From the calculation results (Figure 5a), it can be seen that compared with the model $E_{\text{total}}$, $E_{\text{surface}}$, and $E_{\text{polymer}}$ without the modifier, the number of models containing modifier has increased by 14%, 12%, and 18%, respectively, and $E_{\text{inter}}$ has increased by about eight times. On the one hand, High interaction energy, namely high binding energy, indicates high bond strength between polymer and C-S-H surface [10,31]. Additionally, the interaction energy of the interface is negative, indicating that the combination of the two is an exothermic process and the system is more stable, and it also shows that the modifier can increase the bonding and stability of the interface of EPS concrete. On the other hand, the non-bond energy between the inorganic phase and the organic phase is the sum of the Van der Waals energy and the Coulomb electrostatic force (Figure 5b), which is equivalent to the interaction energy, where the Van der Waals energy increases by 10% and the Coulomb electrostatic force effect increases by about 7 times. This may be because the carbon-hydrogen bonds in EPS alkane molecules are non-polar, and the association is very little, and Alkanes are non-polar molecules in nature and insoluble in water [32]. However, vinyl acetate contains a large number of carboxyl groups (-COOH), which can directly interact with the C-S-H surface through electrostatic attraction, ionic bond and hydrogen bond, etc., enhancing the interaction between the polymer and the crystal plane, resulting in closer bonding, and leading to the increase of the interface adhesion of the composites [33]. This research result is consistent with the findings in the literature [8], which again indicates that the model constructed is reasonable.

### 3.2. Radial distribution function

To further understand the influence of modifier on the interface interaction of EPS concrete, a method of atomic radial distribution function (RDF) is calculated by using the molecular dynamics (MD) method to characterize the adsorption points on the composite
surface of two materials to describe the spatial correlation between atoms [34], which can be used to reveal the interaction mechanism of atoms at the interface. If there is an obvious peak value of RDF between two kinds of atoms, the spatial correlation between them is strong, that is, there is a stable chemical bond [35]. Besides, the inter-molecular forces usually include hydrogen bonding and Van der Waals (Vdw) interaction, which generally ranges from 2.6–3.1 Å for hydrogen bonding and 3.1–5.0 Å for Van der Waals (Vdw), and the Vdw effect is very weak when the effect is greater than 5.0 Å [36]. The calculated radial distribution function of atoms in the study system (as shown in Figure 6).

In the RDF curve of the interface model without the modifier, there is a strong interaction between Ca on the surface of hydrated calcium silicate and C and H on EPS, respectively, while other atoms on the C-S-H surface contribute little to the interfacial bonding strength (Figure 6a). In the RDF curve of the interface model with the modifier, since the peaks formed by most of the interacting atoms in the model with the modifier are not obvious, this paper only shows the atoms with higher peaks formed (Figure 6b). It can be seen from the figure that the curve fluctuation of Ca-C_{EPS} and Ca-C_{EPS} RDF of the interface model with EVA and without EVA is unchanged, but two peaks of the model with EVA are slightly lower than those of the model without EVA. The main reason for this phenomenon is that EVA replaces part of EPS to interact with the Ca atom. What’s more, Ca=O (carbonyl O), Si=O, O_{T}=O, Ca-C_{EVA}, Ca-H_{EVA}, and other interactions are also added to the model containing modifier (Figure 6c), which is found that there is a sharp peak between the carbonyl O in the EVA chain and the Ca atom on the surface of the matrix, which indicates that there is a strong interaction between the two atoms. According to previous research, calcium atoms can bind to oxygen atoms when the distance between oxygen and calcium ions is less than 2.5, which is clear evidence of the formation of ion pairs between O and Ca atoms [37,38]. Oxygen can bridge Ca ions in the C-S-H channel to form a new hydrated calcium silicate gel and fill it into the crack, enhancing the bond between inorganic and organic interfaces [39]. It is also found that the Coulomb electrostatic force is generated by Ca and =O and van der Waals interaction contributes to the enhancement of EVA to the interface interaction between EPS and cement paste.

Combined with the adsorption conformation optimized by kinetics in Figure 4(g) and 4(h), it can be seen that some EVA molecules, due to the electrostatic interaction between the carbonyl group O in the carboxylic acid group and Si and O Coulomb in the C-S-H crystal plane, adsorb on the crystal plane and the C-S-H interface well. Another part of EVA is adsorbed on EPS due to the migration of Ca ions in C-S-H gel to the interface region and the formation of a certain strength ionic bond with the carbonyl group O of EVA. Resulting from the above effects, EVA becomes a bridge for the interaction between EPS and C-S-H, which also well supports the radial distribution function analysis. Therefore, the simulation results can show that EVA enhances the interface interaction, mainly because of the electrostatic interaction between oxygen atoms with double bonds and Ca and O on the cement-based surface. The simulation results are consistent with the research results in the literature [40].

3.3. Mechanical properties

EPS composite concrete is a multi-structure material, containing the interface between the components. This interface plays an important role in the properties of composites, especially mechanical properties. Therefore, in this study, the mechanical properties of the interface model with or without modifiers are calculated to reflect the influence of the
Figure 6. (a) EPS/C-S-H model: the RDF and the snapshot of adsorption conformation. (b)/(c) EPS/EVA/C-S-H model: the RDF and the snapshot of adsorption conformation.
interface surface on the mechanical properties [41]. Mechanical properties refer to the mechanical properties of materials under various applied loads under different environments, in which Young’s modulus, shear modulus, and volume modulus in x, y, and z directions are the main parameters of mechanical properties. Young’s modulus (E) is an index to evaluate the rigidity of a material and a measure of its resistance to elastic deformation. The higher the shear modulus (G) value is, the higher the hardness and yield strength of the material will be, which are measures of the resistance of the material to plastic deformation. The larger the volume modulus (K) value is, the greater the fracture strength of the material will be [10,42]. Using MS to analyze the static elastic mechanical properties of the interface model of pure C-S-H and EPS concrete composites with or without additives under the equilibrium state after optimized annealing, the elastic coefficient matrix of the model can be obtained, and the model can be simplified to isotropic material, which is not extremely heteromorphic material. For isotropic materials, there are only two independent elastic constants in the calculation principle, and then the two Lames coefficients λ and μ are obtained by using the elastic matrix. Finally, each modulus can be obtained by using Eqs. (3)–(5) [43,44].

\[
E = \mu \frac{3\lambda + 2\mu}{\lambda + \mu} \\
G = \mu \\
K = \lambda + \frac{2}{3} \mu
\]

where E is Young’s modulus, G is shear modulus, and K is volume modulus. The mechanical property parameters calculated are shown in Figure 7.

It is found from the results (Figure 7a) that Young’s modulus of EPS/C-S-H is smaller in X, Y, and Z directions than that of pure C-S-H and EPS/EVA/C-S-H. In addition, Young’s modulus of the model containing modifier EVA is close to that of pure C-S-H in three directions. This result is consistent with the macroscopic experimental results. EPS/C-S-H has low Young’s modulus and is difficult to resist large external forces. That is, the interface bond performance is poor. The addition of EVA improves the young’s modulus of the interface, which may be due to the high Young’s modulus of EVA molecules, act

![Figure 7](image-url)
as a bridge for the interaction between EPS and C-S-H, promote the combination of them and increase the interface stability. The order of shear modulus and volume modulus is \( \text{EPS/C-S-H} < \text{EPS/EVA/C-S-H} < \text{pure C-S-H} \) (Figure 7b), which is mainly because EPS concrete contains EPS compressible material, and there is a modulus difference (weak interface) between EPS and cement base. Therefore, the two models cannot achieve the same mechanical properties as pure C-S-H. As has been mentioned above, E, K, and G are measures of material rigidity, and the higher their values are, the stronger the material rigidity is [45]. It shows that the addition of EVA not only retains the excellent characteristics of EPS concrete but also improves its interface mechanical properties. As mentioned above, the interface has a great influence on the overall mechanical properties, so the overall performance of EPS concrete will be effectively improved when the interface performance is enhanced. In addition, this study compared the experimental data of macroscopic cement-based mechanical properties and the results of other papers calculated by the same method and found that there were differences in the calculated mechanical properties parameters, but the overall trend was consistent, which may lead to the differences: (1) The actual research materials are anisotropic materials containing different components. There are many assumptions and simplified calculations in the simulation process of this study. (2) The relaxation method selected by each researcher is different, and the main parameters calculated are different from those in other references. (3) Due to limited computing conditions, it is necessary to rely on supercomputing to get closer to the actual model. However, ordinary computers can only calculate thousands of atoms, so the efficiency is slow and the effect is poor. Due to the above reasons, the simulation results may not be accurate. However, it can be shown that the addition of EPS reduces the mechanical properties of concrete, while the addition of EVA improves the interface mechanical properties of EPS concrete composite materials, and achieves the purpose of energy conservation and environmental protection. It provides basic theoretical support for the application of modified EPS concrete and has reference significance for the future research and development of better quality EPS concrete.

4. Conclusion

In this study, the molecular dynamics simulation method is used to construct the interface model with and without modifiers, and the interaction energy, radial distribution function, and mechanical properties of the two interface models are calculated, and the following conclusions are drawn:

1. Strong interaction exists in the interface model with the modifier. In addition, the interaction energy is approximately equal to the non-bonding energy, which is mainly composed of Van der Waals forces and Coulomb electrostatic forces. The strong interaction may be related to a large number of -COOH polar groups in the EVA chain, which directly interact with the C-S-H surface to improve the bond between EPS and the gel matrix.

2. Through the analysis of radial distribution function, there is a strong interaction between the Ca on the surface of hydrated calcium silicate and the C and H of EPS in the interface model without the modifier. In the model with the modifier, there is not only the former interaction, but also \( \text{Ca-}=\text{O}, \text{O}_1=\text{O}, \text{O}_2=\text{O} \), and other strong interactions, which make EVA act as the bridge between EPS and C-S-H interaction, and play a role in enhancing the interface of EPS/C-S-H.
3. It can be seen from the calculation results of mechanical properties that the addition of EPS reduces the young's modulus (E), bulk modulus (K), and shear modulus (G) of the model, while the above values of the EPS/C-S-H interface model are improved after the addition of modifier. The results show that the rigidity and interface properties are improved. It not only retains the excellent properties of EPS concrete but also improves the interfacial mechanical properties of EPS concrete.

Disclosure statement

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