Mechanical Property Test and Finite Element Simulation Analysis of KH-560 Coupling Agent-Modified PVA Rubber Concrete

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KH-560 coupling agent can significantly improve the cement mortar and the rubber connection interface compatibility problem of poor weak associativity. This is also the problem that rubber concrete cannot be widely used in practical engineering. Therefore, in this study, the improvement of the performance of PVA rubber concrete by the interface modified by KH-560 coupling agent was studied from the aspects of macromechanics, mesostructure, and numerical simulation. The macromechanical test shows that KH-560 coupling agent improves the compressive, flexural, and shear strength of PVA rubber concrete, and the failure mode of the modified PVA rubber concrete also changes from plastic failure to brittle failure. Through FTIR test and SEM observation, it was found that when the rubber concreted is stressed, the PVA fiber and the cement base jointly bear the external force, absorb energy, and play the role of reinforcement. The finite element (ABAQUS) simulation analysis found that the simulated data were similar to the actual test results, and the reliability of the test results was verified by data fitting. The final experimental results of this research have practical guiding significance for the researchers of concrete composite materials to research compression and bending and shearing of test blocks with different dosages. It is used to provide a reliable theoretical basis in the actual engineering.

1. Introduction

In recent years, the global automotive industry has been developing continuously, and the update speed of products has been accelerating. Among them, the problem of “black pollution” caused by waste tires has become the focus on attention on all countries in the world. Under natural conditions, rubber is difficult to degrade, and direct landfill of rubber not only wastes resources and occupies land but also causes great pollution to groundwater. Part of the energy can be recovered by incineration, but it still causes air pollution [1]. At present, the rubber is processed into rubber particles, and the equal volume replaces the fine aggregate in the concrete, that is, rubberized concrete. Today, as part of concrete pouring materials, it has the advantages of good impact resistance, excellent crack resistance, and high toughness, while also recycling waste and improving the environment. Therefore, it has received extensive attention to researchers at home and abroad and has been gradually applied to engineering [2].

At present, domestic and foreign scholars basically focus on mechanical properties, durability, and structural applications. Wang et al. [3] introduced polyvinyl alcohol (PVA) fibers to improve the performance and durability of rubberized concrete, indicating that PVA fiber-reinforced rubberized concrete can improve the durability and ductility of cementitious materials for structural construction. Both Liu et al. and Zhou et al. [4, 5] put forward the idea of hybrid fiber reinforced concrete (HFRC) to improve the mechanical properties of concrete. Through a series of macro- and microscale tests, and combined with the analysis of the relationship between the microstructural characteristics and mechanical properties of HFRC, the final results show that steel fibers can improve the mechanical properties of HFRCF. Liu et al. [6] studied the tensile strength of the modified materials with different mixing ratios (steel : PVA = 1 : 3 ~ 3 : 1) and fiber volume
content (1%–3%), and captured the test with digital image correlation (DIC) measurements. During the crack formation and propagation, the results show that the tensile strength of HFRC increases with increasing steel fiber content and decreases with increasing PVA fiber content. Li et al. [7] studied the effect of fiber content on the shear strength and toughness of HFRC. The test showed that the concrete containing 180 kg/m² steel fibers and 4.5 kg/m² basal fibers performed the best in terms of shear strength and toughness. Liu et al. [8] used silane coupling agent (SCA) to modify the surface of the steel fiber to enhance the bonding between the fiber and the matrix. The results show that the modification of steel fibers with SCA can improve the interfacial adhesion and tensile properties of UHPC. Manca et al. [9] proposed a method based on image processing and machine learning to capture digital images of fractured surfaces to obtain fiber distribution. Pujadas et al. [10] focused on the structural response to the hypostatic concrete slab reinforced with plastic crude fiber and obtained the constitutive model of the plastic fiber reinforced concrete by using experimental research and numerical simulation. Yuan et al. [11, 12] used a glass fiber-modified polyvinyl alcohol (SH polymer) to strengthen granite residual soil and used scanning electron microscope (SEM) to observe the microscopic interaction mechanism and impact performance of granite soil, and then analyzed the reinforcement effect of glass fiber. In view of the weak interface between the expanded polystyrene and concrete, Feng et al. [13] discussed the interface strengthening mechanism through molecular dynamic simulation on the basis of macroscopic experiments and concluded that EVA plays a role as a bridge between EPS and C-S-H. Li et al. [14] studied the feasibility of applying rubber concrete to highways and railways, showing that rubber concrete has good noise reduction, ductility, and heat preservation and is suitable for practical engineering. Yuan et al. [15] studied the layered soil displacement of transparent soil laterally loaded piles and observed the layered soil displacement more intuitively through the visualization method. Yu et al. [16] studied silane coupling agent to modify rubber hydrated calcium silicate, used molecular dynamics to simulate and analyze, and finally concluded that the addition of silane coupling agent greatly changed the water molecular structure at the interface between rubber and silane. Han et al. [17] proposed a new surface treatment method using PVA to improve the hydrophilicity of waste rubber, and verified the bridge role of PVA at the molecular scale. Chou et al. [18] proposed the idea of using waste organic sulfur compounds as raw materials to modify the surface of rubber particles and concluded that organic sulfur compounds can improve the mechanical properties of rubber concrete. Wang et al. [19] discussed the synergistic effect of polypropylene fiber and rubber concrete from the aspects of mechanical properties, durability, microstructure, etc. The results show that polypropylene fiber can enhance the durability and frost resistance of rubber concrete. Thomas and Chandra [20] studied the applicability of waste tired rubber as a natural fine aggregate of concrete, tested the compressive strength, tensile strength, pullout strength, and wear resistance of concrete, and observed its structure of scanning electron microscope (SEM).

The above research has promoted the wide application of rubberized concrete in practical engineering, and the research on its mechanical properties mainly focuses on the compressive and split tensile tests. However, in the actual project, the rubber concrete may also be subjected to shear force, so this experiment also adds a shear test. In this study, KH-560 coupling agent is used to modify the interface between PVA and cement base, and the interface between rubber and cement base. The coupling agent acts as a bridge between rubber raw materials, PVA, and cement paste and improves the interface bond strength of composite materials. And the macroscopic mechanical test, scanning electron microscope (SEM), infrared spectroscopy (FTIR), and finite element simulation analysis methods were used to study the influence of KH-560 coupling agent on the PVA rubber concrete interface at different levels. The technical route of this study is shown in Figure 1.

2. Indoor Material Parameters and Raw Material Mix Ratio

2.1. Materials. The raw materials used in this experiment include PVA fibers, stones, sand, rubber particles, cement, and KH-560 coupling agent, as shown in Figure 2.

The cement used in the concrete was provided by China United Cement Co., Ltd. (Hebei, China). P.O42.5 ordinary Portland cements were selected with a strength of 42.5 MPa. The main chemical components are shown in Table 1. Provided by the company, the physical properties are shown in Table 2. KH-560 coupling agent was provided by Jinan Xingfeilong Chemical Co., Ltd. The physical properties are shown in Table 3; the basic information on rubber particles is shown in Table 4; the fine aggregate is river sand, the fineness modulus is 2.5, the apparent density is 2650 kg/m³, and the bulk density is 1850. Coarse aggregate is a continuously graded (5~25 mm) crushed stone, the bulk density is 1550 kg/m³, the apparent density is 1703 kg/m³, and the rubber substitution rate is calculated by the method of replacing fine aggregate by equal volume (R₁). R₁ is the rubber particle content when the rubber substitution rate is 0%, 5%, 10%, and 15% respectively. The PVA fiber was directly added in equal volume, and its substitution rate R₂ was 0.5%, 1%, and 1.5% respectively, and the amount of coupling agent added was 1.5% of the total volume. The specific coordination of each material is shown in Table 5. The compressive test, shear test, and flexural test were carried out on the rubber concrete specimens with different rubber substitution rates. C30 was the reference concrete, and its design strength was 30 MPa.

2.2. Sample Preparation. Refer to JGJ55-2011 “Ordinary Concrete Mix Proportion Design Regulations” [21] to determine the concrete mix ratio, take PVA, KH-560 coupling agent, and rubber content as controllable factors, and use equal volume to replace fine aggregate to calculate the rubber replacement rate. PVA fiber and coupling agent are directly added according to the same volume, and the specific coordination is shown in Table 5.
The mechanical properties were tested according to “Standard Test Methods for Fiber Reinforced Concrete” [22] (CECS 13:2009). The compressive, flexural, and shear dimensions of the test block are 100 mm × 100 mm × 100 mm, 40 mm × 40 mm × 160 mm, and 150 mm × 150 mm × 150 mm. The specific process is as follows: Step 1: preparing for the work and preparation for the mold test: clean the test mold, brush the coating agent evenly on the inner surface, and place a thin paper on the bottom hole. Step 2: put the cement, sand, PVA fiber, rubber particles, stones, and water+silane coupling agent into the mixer for mixing, put the concrete into the test mold, put it on the vibrating table and vibrate, and continue to produce slurry on the concrete surface. So far, the slump greater than 70 mm is manually tamped, and finally, a spatula is used to insert and pull along the inner wall of the test mold several times. Step 3: after molding, use standard curing specimens for 28 days. Step 4: remove the mold and write the number with a pen after the specimen is condensed. Compression, shear, and flexural tests were performed on the specimens. The loading rate determined according to GB/T50081-2002 “Standards for Mechanical Properties of Ordinary Concrete” is 0.5~0.8 MPa/s. The shear test adopts the displacement loading control method, and the loading rate is 1 mm/min.

3. Comparative Analysis of Macroscopic Mechanical Test and Mesoscopic Test

3.1. Analysis of Pressure Test Results. According to the concrete uniaxial compression test scheme, the compression
failure morphology of concrete before and after modification with silane coupling agent and the stress-strain curves of different dosages are shown in Figures 3 and 4.

Under different substitution rates of rubber and PVA, crack surfaces approximately parallel to the direction of compressive loading were formed into the side of the specimen, and the failure forms were similar. The difference is that the KH-560 coupling agent is added in the same mixing ratio, and it can be clearly seen that the cracks are reduced and the compressive capacity is enhanced. The analysis shows that the reason for the insufficient strength of rubberized concrete is that cement mortar is a hydrophilic material, while rubber is a hydrophobic material, so the compatibility and interface bonding ability are poor when mixed and used. The cracks were larger and the concrete fell off. After adding KH-560 coupling agent, the number of concrete cracks is reduced, and the crack width is reduced. It can be seen more intuitively from the macroscopic mechanical test that the modification of rubber by silane coupling agent can significantly improve the bonding performance of the two.
Under different rubber and PVA substitution rates, the development trend of stress-strain curves of each specimen is basically the same. With the continuous increase in the load, the stress failure of the concrete block develops from the elastic stage to the elastic-plastic stage. When the load reaches the concrete failure load, the curve begins to enter the descending stage. At the same time, the stress-strain curve of the specimen has good continuity and smoothness, but with the increase of the admixture substitution rate, the compressive strength of the specimen decreases obviously.

Extract the characteristic value of the stress-strain curve (peak compressive strength) of Figures 4(d), 4(e), and 4(f); the peak compressive strengths of rubber concrete with different contents are as follows: C30 is 27.02 MPa, CRC 5%-PVA 0.5% is 22.51 MPa, CRC 5%-PVA 1.0% is 22.01 MPa, CRC 5%-PVA 1.5% is 21.04 MPa, CRC 10%-PVA 0.5% is 19.56 MPa, CRC 10%-PVA 1.0% is 18.52 MPa, CRC 10%-PVA 1.5% is 17.89 MPa, CRC 15%-PVA 0.5% is 17.54 MPa, CRC 15%-PVA 1.0% is 17.20 MPa, CRC 15%-PVA 1.5% is 16.54 MPa, CRC 5%-PVA 0.5%-KH-560 is 26.42 MPa, CRC 10%-PVA 1.0%-KH-560 is 23.45 MPa,

Figure 4: Stress-strain curve of compressive test block.
and CRC 15%-PVA 1.5%-KH-560 is 22.51 MPa. The analysis of these characteristics is worth the conclusion: with the increase in the substitution rate of rubber, PVA, and KH-560 coupling agent, the uniaxial compressive strength of the specimens decreases to different degrees.

With the increase in rubber content, the peak value of compressive strength gradually decreases. The data analysis is as follows: when the PVA content is 0.5%, 1.0%, and 1.5%, respectively, the rubber content is 5%, 10%, and 15%, and the compressive strength of rubber concrete is decreased by 22.07%, 21.85%, and 21.39%, respectively. That is, when the PVA fiber content is the same, with the increase of the rubber content, the compressive strength gradually decreases; when the CRC particle content is 5%, 10%, and 15%, respectively, the PVA content is 0.5% and 1.0%. At 1.5%, the compressive strength of rubber concrete is decreased by 6.53%, 8.54%, and 5.7%, respectively. That is, when the CRC content is the same, with the increase of the PVA content, the compressive strength gradually decreases; when CRC 5%-PVA 0.5%, CRC 10%-PVA 1.0%, and CRC 15%-PVA 1.5%, KH-560 doping the compressive strength of rubber concrete increased by 17.37%, 26.62%, and 36.09%, respectively, when the amount was 0% and 1.5%. That is, when the contents of PVA and CRC are the same, the addition of KH-560 coupling agent can improve the compressive strength of concrete blocks.

3.2. Analysis of Flexural Test Results. The DKZ-5000 electric flexural testing machine was used to carry out the flexural test, and the flexural failure mode of each specimen and the bar graph of the shear strength of each specimen were obtained.

It can be seen from Figure 5 that the failure patterns of the rubber concrete specimens with different contents are similar, and they are all fracture failures in the middle of the specimens. The reason is that under the action of the breaking equipment, when the concentrated stress reaches the ultimate bearing capacity of the concrete, the specimen breaks and fails. The difference is that with the increase in the rubber substitution rate, the fracture surface of the specimen becomes more and more uneven, and the fractured surface also increases from a small amount of rubber particles. The flexural strength of concrete is an important index to measure the quality of cement concrete pavement, and the main factors affecting its flexural strength are the mix design and sand ratio of materials. The flexural strength is shown in Figure 6.

It can be seen from Figure 6 that when the PVA fiber content is 0.5%, 1.0%, and 1.5%, the rubber content increases from 5% to 10%, and the flexural strength of rubber concrete increases by 14.78%, 25.43%, and 33.60%, respectively. With the increase of PVA content, the flexural strength is gradually increased.

3.3. Analysis of Shear Test Results. The instrument used in the shear test is a Y250 digital-display electromechanical stress-type direct shearing instrument. The pure shear stress failure forms and shear bar graph of each specimen obtained are shown in the following figures.
It can be seen from Figure 7 that the cracks of the specimen perpendicular to the shearing direction are relatively straight, while the cracks parallel to the shearing direction are irregular in shape. The shear failure section of the specimen is relatively similar, the shear plane is relatively uneven, and there is a small amount of concrete debris. The larger the rubber substitution rate is, the more rubber particles fall off on the shear failure section of the rubber-concrete specimen.

It can be seen from Figure 8 that the pressure is 2.22 MPa. When the CRC content is 5%, 10%, and 15%, and the PVA content increases from 0.5% to 1.5%, the shear strength of the rubberized concrete decreases by 5.95%, 4.78%, and 6.19%, respectively. That is, when the content of CRC is the same, with the increase of the content of PVA, the shear strength of rubber concrete decreases gradually. When CRC 5%-PVA 5%, adding coupling agent increased shear strength by 10.21%; when CRC 10%-PVA 1.0%, adding coupling agent increased shear strength by 10.55%; when CRC 15%-PVA 1.5%, adding coupling agent increased shear strength by 10.97%. Therefore, it can be concluded that when CRC 15%-PVA 1.5%, adding coupling agent has the best effect.

Under the action of two different normal forces, 2.22 MPa and 4.44 MPa, the development trend of the pure shear force histogram of each specimen is basically the same. With the increase of the rubber substitution rate, the shear failure load of the rubber concrete specimen gradually decreases, the reason is that the increase in the replacement rate of rubber particles weakens the shear failure section of the rubber concrete specimen, and at the same time, the bonding performance between rubber particles and cementitious materials, rubber particles, and crushed stone is poor, so that the shear of the failure load gradually decreased with the increase of the rubber substitution rate; in addition, under the same rubber particle substitution rate, with the increase of the PVA fiber substitution rate, the shear load of the rubber concrete specimen gradually increased; because the addition of PVA fiber is just like adding fiber reinforcement in concrete, these fiber reinforcements inhibit the cracking process of concrete and improve
Figure 7: Shear failure morphology of specimens with different dosages.

Figure 8: Shear force histogram of different dosages when the normal force is 2.22 MPa.
the fracture toughness of concrete. Produce mutually restrained shear stresses. It can also be found that the addition of the coupling agent can enhance the shear strength of the rubber concrete to a certain extent, because the silane coupling agent used can improve the adhesion between organic and inorganic substances, so that the two can be better. Resist external forces together.

3.4. Summary of Macroscopic Mechanic Experiments. According to the composition characteristics of PVA rubber concrete, the rubber particles are simplified into a circular particle model as shown in the figure, and PVA is simplified into a linear object as shown in the figure. Considering the different loading methods of the test, the action mechanism of PVA rubber concrete is analyzed.

As mentioned above, with the increase of the replacement rate of rubber particles, the compressive strength, flexural strength, and shear strength of PVA rubber concrete gradually decreased; under the same rubber particle content, with the increase of PVA fiber content, the compressive strength of the concrete test block is gradually reduced, but the flexural strength and shear strength are improved in different degrees; through the comparative analysis before and after the addition of the silane coupling agent, it can be seen that the silane coupling agent can significantly improve the compressive, flexural and shear strength of rubber concrete specimens. From the failure modes of rubber concrete with different loading methods, it can be seen that the rubber concrete with different rubber and PVA substitution rates is under compression, and the failure mechanisms of shear and bending are the same, as shown in Figure 10.

During the preparation and solidification process of rubber PVA fiber concrete, the water loss and shrinkage of the cement slurry is larger than that of the coarse aggregate, resulting in the formation of a stress field on the cross-section, and the local stress may be so large that microcracks occur at the aggregate interface. At the same time, when the cement in the concrete produces hydration heat or the environment changes, the temperature stress field is formed due to the difference in temperature deformation. At the same time, the concrete is a thermally inert material, and the temperature gradient greatly increases the temperature stress. This part is a microscopic factor. Rubber PVA fiber concrete has a small amount of microcracks before it is loaded. First, the cement mortar forms microcracks along the coarse aggregate interface and inside the mortar; as the stress increases, the microcracks expand into macrocracks; the rubber cannot provide mechanical force during the stress process. The strength of the concrete is reduced, and the performance of the concrete is reduced; the PVA fiber plays a role in strengthening the tie in the concrete and can provide higher crack resistance when the concrete is damaged by

![Figure 9: Shear force histogram of different dosages when the normal force is 4.44 MPa.](image-url)
force. Eventually, the damage to the mortar builds up severing the connection with the aggregate until the concrete fails and loses its bearing capacity.

The characteristics of concrete materials, whether under compression, shear or bending, there is chemical adhesive force between mortar and mortar and between mortar and coarse aggregate. This effect is mainly related to the composition characteristics of mortar. When the particle substitution rate increases, the bonding force between the rubber and the mortar is relatively weak. On the other hand, the compressive capacity of the rubber particles is much smaller than that of the fine aggregate, and the deformation capacity is higher than that of the fine aggregate, which finally makes the rubber concrete. The mechanical performance is reduced, and the deformation capacity is gradually improved. At this time, PVA fibers are added to act as reinforcing bars, and silane coupling agent is used to enhance the interfacial adhesion between rubber, PVA, and cement and finally improve the mechanical properties of rubber concrete specimens and retain the good modification of the specimens’ ability.

3.5. Scanning Electron Microscope (SEM). A scanning electron microscope was used to observe the interface of different materials of the specimen, and the equipment was Quanta FEG produced by Beijing Zhuotong Technology Co., Ltd. The target sample was cut into cubes of 10 mm × 10 mm × 10 mm, polished with a 2000-grit sandpaper, and ultrasonically cleaned with absolute ethanol to remove surface powder impurities. The cleaned samples were tested after drying at 60 ± 2 °C for 5 h.

Figure 11 is the scanning electron microscope image of the interface of the specimen modified by KH-560 coupling agent. It can be clearly seen that KH-560 improves the bonding effect of organic matter and inorganic matter. It is observed in Figure 11(a) that the interface between the cement base and the rubber particles is almost in a separated state, and there are many loose network structures in the interface, indicating that the cement base and the rubber are poorly bonded and the interface is hydrated. The degree of unevenness is not uniform, and the interface is relatively fragile, so the specimen will be damaged in advance when it is stressed. After adding 1.5% KH-560 coupling agent, as shown in Figure 11(b), it can be clearly observed that the interface between cement and rubber has no obvious cracks, and the bonding is tight, forming a continuous and uniform interface. The hydrophobicity of the rubber particles makes the hydration reaction of the surface area lack, so cracks are generated in the transition area between rubber and concrete, and stress concentration is caused at the same time, which becomes the weak point of the material. After adding a coupling agent for modification, the hydration products can be induced to grow and accumulate at the rubber interface, and the cracks in the modified interface area are filled with cement hydration products. Although the structure is relatively loose, compared with the unmodified rubber, the modification treatment greatly improves the hydration of the cement in the interface area between the rubber and the cement, thereby effectively repairs the interface defects between the rubber and the hydration product. Figures 11(a) and 11(b) show that KH-560 can significantly improve the bonding force between cement base and rubber, thereby improving the mechanical properties of rubber concrete. It can be seen from Figure 11(c) that when the cement matrix and PVA fibers work together, the interfacial connection is loose, the cohesion is poor, and the PVA and cement particles undergo chemical reactions to produce new hydration products and form a continuous network polymer. The membrane reduces the pore size inside the concrete, so that the PVA fiber cannot fully play the role of the steel bar. In Figure 11(d), after KH-560 modification, the connection between PVA fiber and the cement matrix is more tight, and its film-forming effect is used to improve the structure of the interface transition zone of concrete. By reducing the thickness of the transition zone, the hardness is improved. To improve the bond strength of aggregate and mortar, the interface properties are improved. It can better exert the ductility of PVA, reduce the brittleness of PVA rubber concrete, and improve the ductility. This is also

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Figure 10: Concrete failure mechanism with different loading methods.
the reason why the PVA rubber concrete shedding material is reduced after adding KH-560 coupling agent in the macrotest.

3.6. Infrared Spectrum (FTIR). Considering that the interface after modification may affect the functional group changes, further analysis of the chemical effect of KH-560 coupling agent in the cement hydration process is required. In this study, a PerkinElmer PE spectrum two infrared spectrometer was used to conduct infrared spectrum analysis on target specimen, and the KH-560 coupling agent was tested by a liquid cell. The resolution of the test is 4, the wave number range is 4000~500, and the number of scans is 32 times. By observing the formation and disappearance of characteristic functional groups of the samples before and after modification, the modification status of the interface between PVA fibers, rubber particles, and cement matrix was qualitatively analyzed.

Silane coupling agent KH-560 is a low-molecular-weight organosilicon compound with the general formula RSiX₃, where R represents an active functional group that has affinity or reactivity with polymer molecules and X represents a hydrolyzable group. When KH-560 is used for coupling, the X group forms a silanol and reacts with the hydroxyl group on the surface of the inorganic substance to form a hydrogen bond and condense into a SiO–M covalent bond. The silanols of the silane molecules are polymerized into a network-like film attached to the surface of the particles, which makes the surface of the inorganic powder organic.

The coupling agent may have an effect on the type and quantity of functional groups at the rubber-cement interface and the PVA-cement interface. It can be seen from the above figure that the corresponding characteristic value of the coupling agent appears on the surface of the modified rubber particles, and it is found that the vibration band of the infrared spectrum with KH-560 coupling agent is weaker than that without KH-560 coupling agent, accompanied by the appearance of a small number of peaks. CRC+PVA in Figure 11 shows the infrared spectrum of the cement wrapped on the surface of the original PVA rubber particles. The absorption at 3318 is the stretching and bending vibrations of -OH, and the absorption peak at 880 represents the stretching vibration of the Si-O bond between C-S-H. The absorption peaks at 1088 and 1046 correspond to the vibration peak, respectively, which originate from the presence of cement particles of hydration. In addition, the band appearing around 2973 is attributed to the organic chain of the rubber. The band appearing around 2973 is attributed to the organic chain of the rubber. CRC+PVA+KH-560 in Figure 12 shows two small absorption peaks at 2879 and 3323 in the infrared spectrum curve of the coupling agent after successful modification, because the chemical environment of the hydroxyl group in the sample has changed after the modification of the coupling agent, which is very likely due to the reaction between siloxane oligomers and cement hydration products. The siloxane oligomers form hydrogen bonds with the hydroxyl groups of C-S-H and CH in cement during cement hardening. The absorption peak at 1379 in the spectrum is related to the Si-O-Si pull-up of siloxane oligomers, indicating the possibility of hydrolytic condensation reaction to coupling agent molecules. It can be said that the coupling agent molecule forms an intermediate with one, two, or three hydroxyl groups after hydrolysis, and then, the intermediate shrinks and reacts to form a siloxane oligomer, which contains Si-O-Si chemical bonds [23]. Therefore, the bonding force of
the interface between organic matter (rubber and PVA) and inorganic matter (cement) is improved, so that the mechanical properties of PVA rubber concrete are improved.

4. Finite Element Simulation Analysis

4.1. Basic Assumptions. Assumptions are as follows: (1) Concrete is a homogeneous continuous material. (2) The distribution of rubber particles and PVA fibers in the concrete matrix is uniform. (3) The particle size of rubber particles is small and can be approximately regarded as spherical. (4) The distribution of PVA fibers is approximately linear. (5) The interaction between adjacent particles can be ignored.

4.2. ABAQUS Modeling Process Based on Python Language. Considering the limitation of the modeling function of ABAQUS software, based on finite element calculations, a Python script is written to generate points that are uniformly scattered over time in a specified area and then generate arbitrary directions over time from these points. The line element completes the creation model of the fiber element. At the same time, a Python script was written, and the uniform distribution function of the NUMPY function library was used to simulate the random delivery process of particles. Run these two scripts simultaneously in ABAQUS to uniformly distribute the rubber particles and PVA fibers in the concrete at the same time, realize the rapid establishment of the composite material model, and improve the efficiency of composite material analysis. Based on the above assumptions, a model with a size of $100 \text{ mm} \times 100 \text{ mm} \times 100 \text{ mm}$ is created through the secondary development of Python in ABAQUS for simulation experiments. The PVA rubber concrete model is shown in Figure 13.
Figure 14: Continued.
The concrete test block is composed of mortar matrix, polyhedral aggregates, rubber particles, PVA fibers, the interface of mortar matrix and polyhedral aggregates, the interface with mortar matrix and rubber particles, and the interface of mortar matrix and PVA fibers. In order to facilitate modeling and improve calculation, in this paper, the concrete mortar matrix and the polyhedral aggregate are homogenized for the time being, and the interface part is also ignored first. Referring to the work of Masad et al. [24], in the finite element analysis of this paper, the concrete matrix adopts the plastic damage model, and the compressive stress-strain relationship of concrete under monatomic load adopts the model proposed by Popovics [25].

The expansion angle is taken as 32°, the eccentricity is taken as 0.1, the ratio of biaxial to uniaxial compressive strength is taken as 1.16, the coefficient K is taken as 2/3, and the viscosity coefficient is taken as 0.005. The mechanical parameters of different materials are shown in Table 6.

4.3. Comparison of Stress Distribution with Experimental Results. Based on the above finite element method, as shown in Figure 14, the uniaxial compression failure simulation of concrete cubes of different ratios was carried out. Figure 15 plots the stress-strain curves of the specimens under compression. It can be found that with the addition of rubber particles and PVA fibers, the uniaxial compressive strength of concrete shows a downward trend, which is basically consistent with the experimental trend, and the overall law is basically consistent with the law summarized above. However, in the actual fiber-
Figure 15: Continued.
reinforced concrete, the addition of fibers will inevitably lead to more air entering the concrete matrix, and aggregation will occur under the action of the coupling agent, so the overall performance of the fiber-reinforced concrete will be improved in the simulation.

5. Conclusions

The macroscopic tests conducted in this study investigated the influence of KH-560 coupling agent modification on the mechanical properties of PVA rubber concrete. The effect on the surface hydration and functional groups of PVA cement was analyzed by FRIT. The effect of KH-560 coupling agent on the microstructure of PVA cement-based interface was observed by SEM. The compressive condition of the simulated specimen is fitted with the actual compressive condition by finite element (ABAQUS), which provides the basis for the test conclusion. Based on the results of the study, the following conclusions can be drawn:

(1) The results of macroscopic mechanical properties showed that the compression test, shear test, and flexural failure mechanism of rubber concrete with different rubber substitution rates are the same, independent of rubber substitution rate. When the admixture of PVA fibers and rubber particles increased, the compressive strength of the specimens decreased to varying degrees, but the flexural strength increased with the increase of PVA fibers. Meanwhile, the surface modification of KH-560 coupling agent can effectively improve the mechanical properties of PVA rubber concrete.

(2) The results of FITR analysis showed that the KH-560 coupling agent delayed the hydration of cement and reduced the generation of Ca(OH)₂, which is detrimental to the mechanical properties. On the contrary, the addition of KH-560 coupling agent increased hydrated calcium silicate and optimized the composition of the interface cement hydration products, thus enhancing the bond of the rubber, PVA, and cement interfaces.

(3) According to SEM observation, the physical and chemical differences between rubber and cement base lead to obvious gaps in the interface of rubber/cement paste, and the physical and chemical differences between PVA and cement base resulted in obvious porosity at the interface between the two, and the addition of KH-560 coupling agent significantly increased the densities and attenuated the interfacial effects at the interface between PVA, rubber particles, and cementitious base.

(4) The finite element software simulations showed that the compressive model created by the finite element software shows that the elastic modulus of the rubber particles is lower in the mesoscopic level, and the strain of the rubber particles is larger than that of the mortar aggregate when subjected to the same external force. The stress damage of the specimen is first concentrated around the rubber particles, and then expanded and formed, and finally developed into an initial crack. PVA fiber can act as a bridge to reduce plastic shrinkage cracks in concrete.
Data Availability

No data were used to support the study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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