A New 3D Meso-mechanical Modeling Method of Coral Aggregate Concrete Considering Interface Characteristics

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Abstract: On the basis of the three-dimensional (3D) random aggregate & mortar two-phase mesoscale finite element model, C++ programming was used to identify the node position information of the interface between the aggregate and mortar elements. The nodes were discretized at this position and the zero-thickness cohesive elements were inserted. After that, the crack energy release rate fracture criterion based on the fracture mechanics theory was assigned to the failure criterion of the interface transition zone (ITZ) elements. Finally, the three-phase meso-mechanical model based on the combined finite discrete element method (FDEM) was constructed. Based on this model, the meso-crack extension and macro-mechanical behaviour of coral aggregate concrete (CAC) under uniaxial compression were successfully simulated. The results demonstrated that the meso-mechanical model based on FDEM has excellent applicability to simulate the compressive properties of CAC.

Key words: coral aggregate concrete(CAC); finite discrete element method; 3D meso-mechanical model; fracture cracks; C++

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0 Introduction

Since the "Ocean Power" strategy was proposed, the need for island construction in the South China Sea has become increasingly urgent. This has also stimulated a huge demand for raw concrete materials such as stone, sands and fresh water. All of them are scarce resources on the islands and need to be transported from the mainland. To reduce transportation costs and facilitate the project schedule, coral aggregate concrete(CAC) made from coral aggregates mined from seawater has great potential in the field of coral reef construction[1].

To evaluate the static mechanical properties of CAC, Yu et al.[2-5] systematically investigated the basic mechanical properties of CAC such as compressive strength, and splitting tensile strength from engineering design requirements. However, it is not possible to reveal the internal damage mechanism of CAC through experiments or homogeneous models, and it is difficult to establish the relationship between the properties of each component material and the macro-mechanical properties. Therefore, it is essential to further investigate the mechanical properties of CAC on a mesoscopic scale.

With the development of computer technology and numerical analysis methods, many scholars have proposed various meso-mechanics methods to analyze the mechanical response and damage mechanism of concrete under different loads, including the theoretical analysis method, the finite element method (FEM)[6-7], the discrete element method (DEM)[8-9] and the extended finite element method (XFEM)[10]. CAC is generally considered to be composed of coral mortar, coral aggregate and ITZ at the mesoscopic scale. But the mesoscale

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model built around CAC now does not provide a complete description of the mechanical model of ITZ. Wu et al.[11-12] constructed a meso-mechanical model of CAC based on the FEM, regarding ITZ as a continuum damage plastic model, and the material parameters as empirical values. The geometric dimensions of ITZ also differs greatly from the reality, and it is difficult to guarantee the accuracy of the numerical calculation results. In a nutshell, the rational characterisation of the mechanical properties of real CAC is essentially a study of the realism of the mesoscale model and the accuracy of the material constitutive relationship. In this paper, based on the fracture mechanics theory, zero-thickness cohesive elements[13] are introduced to characterise the geometry and mechanical properties of ITZ. Combining the advantages of FEM and DEM, as shown in Fig.1, the finite element-based analysis of continua of coral aggregate and mortar is merged with discrete element-based contact interaction solutions between the two (ITZ constitutive equation). A new 3D meso-mechanical model of CAC considering interface characteristics is constructed based on FDEM[14], and the feasibility of the model is verified by the results of CAC uniaxial compression tests.

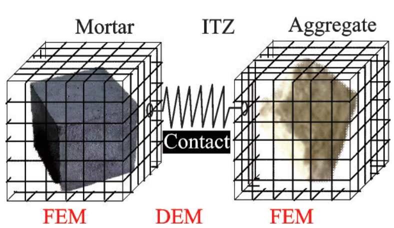

Fig.1 Model of coral aggregate, mortar and ITZ based on FDEM

1 3D Mesoscale Modeling Algorithm

The 3D mesoscale model generation algorithm was carried out in two main steps. The first step was an aggregate & mortar two-phase FEM model generation algorithm. The second step was the cohesive elements embedding algorithm to characterise the bonding effect of ITZ. Finally, the three-phase meso-mechanical FDEM model containing aggregate & mortar & ITZ was generated.

1.1 Random aggregate & mortar two-phase mesoscale FEM model generation algorithm

To establish a 3D random aggregate model without concave corners and flaky features, based on a spatial octahedral aggregate matrix, a shape control technique was used for random growth of polyhedra in space to avoid sharp corners and flaky aggregates, and the vector discriminant algorithm was used to determine random polyhedral convexity. In order to satisfy the random distribution properties of aggregates in concrete, the aggregate placement was performed to adopt the take and place algorithm[15], resulting in the physical model of random convex aggregates. Based on the mapping grid algorithm, the physical model was divided to obtain a homogeneous finite element grid, and the aggregate & mortar two-phase finite element meso-mechanical model was generated by identifying and assigning the material properties of each mesoscopic component[16-17]. The algorithm diagram of this step is shown in Fig.2.

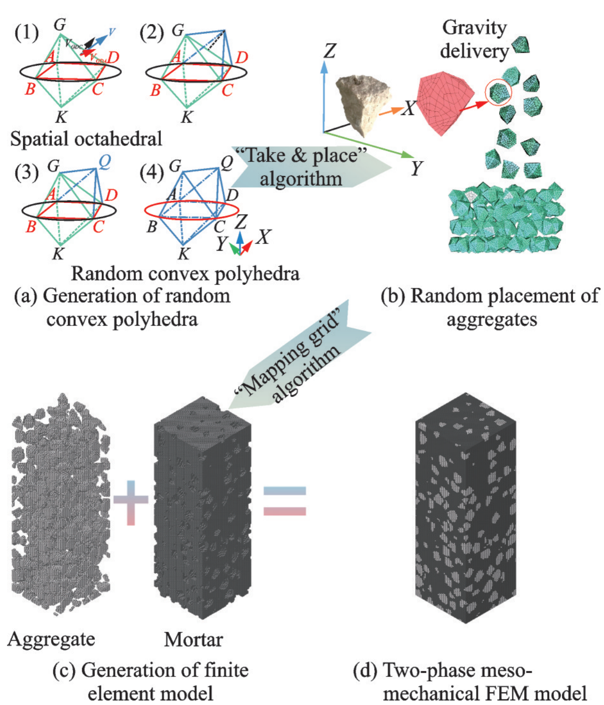

Fig.2 Two-phase mesoscale FEM model generation algorithm

1.2 Cohesive element embedding algorithm

The cohesive elements embedding algorithm is based on the above aggregate & mortar mesoscale FEM model. Firstly, the element and node data of the aggregate and mortar were analysed by C++ programming. Secondly, the interface nodes were identified by the intersection algorithm. After that the aggregate elements and mortar elements were discretized at the interface location. Finally, the new coincident nodes were generated at that location to create cohesive elements. The above description implements the insertion of the zero-thickness 3D cohesive elements into the two-phase mesoscale model to characterize the contact interaction between the aggregate and the mortar, and establishes an aggregate & mortar & ITZ three-phase mesoscale FDEM model. The algorithm for this step is shown in Fig.3.

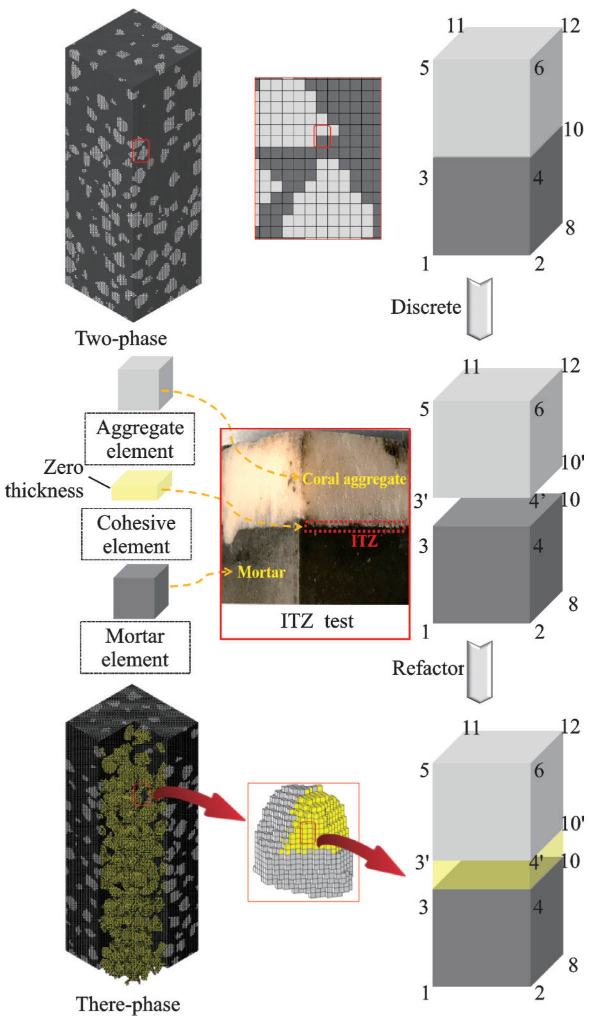

Fig.3 Three-phase mesoscale FDEM model generation algorithm

2 CAC Uniaxially Compressed Mesoscale Simulation

On the basis of the 3D concrete mesoscale FDEM model, the material mechanics models for mesoscopic components of concrete were introduced, and the uniaxial compression test results of CAC were used to verify the applicability of the meso-mechanical model established in this paper. On this basis, the fracture damage process of CAC under uniaxial pressure load was analysed.

2.1 Mesoscale model validation

Based on the model generation algorithm compiled in the previous section, a prismatic model of 100 mm×100 mm×300 mm was established according to Ref.[18]. Then polyhedra were placed according to the coral coarse aggregate gradation in the test with a maximum aggregate size of 20 mm and a volume fraction of 23.2%. The element size of the established FEM model was 2 mm and the total number of hexahedral elements was 375 000. The C++ algorithm program was used to discretize the interface nodes and insert cohesive elements at the location, the number of ITZ elements was 111 356 after insertion. The iso-strain monotonic loading method was adopted, and the loading strain rate was 2×10^{-6} s^{-1}. Further, the friction coefficient was set to 0.9 on the loading end face to simulate boundary constraints. The actual test and numerical test diagrams are shown in Fig.4.

The Karagozian & Case (KC)[19] material model and the Johnson-Holmquist-Concrete (JHC)[20] material model, which characterize the compressive properties of concrete materials, were used for mortar and aggregate elements, respectively, to represent the complex non-linearity of the mechanical behaviour of mortar and aggregate elements when compressed. ITZ adopted a Cohesive_General[13] material model based on the theory of interfacial fracture mechanics, considering a mixed fracture failure criterion[21] and a bilinear softening curve[22] as the constitutive model. The main material model parameters are shown in Table 1. The mechanical

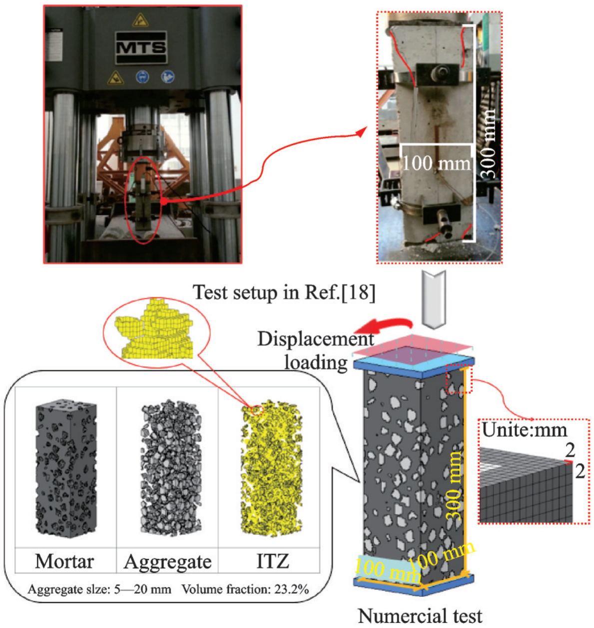

Fig.4 Test in Ref.[18] and mesoscale model simulation test

parameters of coral aggregate and coral mortar referred to the test results in Refs.[23-24], the empirical formulae for bond strength of ITZ referred to that in Refs. [25-26], and the remaining fracture toughness parameters referred to the coral aggregate-mortar interface tests[27-28]. These are described as

$$f_{\text{ts-ITZ}} = 1.012\,7 f_{\text{ts}} - 0.398\,3 \quad (1)$$

$$\tau_{\text{ITZ}} = 7 \times f_{\text{ts-ITZ}} / 4 \quad (2)$$

$$G_{\text{II}}^{\text{C}} = 10 G_{\text{I}}^{\text{C}} \quad (3)$$

where $f_{\text{ts-ITZ}}$ is the interfacial splitting tensile strength (MPa); f_{ts} the net cement mortar splitting tensile strength (MPa); and τ_{ITZ} the interfacial shear strength (MPa). G_{I}^{C} and G_{II}^{C} are the system critical energy release rates for mode Ⅰ and Ⅱ, respectively.

Table 1 Material parameters for CAC components

Component	Mass density/ (kg·m^{-3})	Compressive strength/MPa	Tensile strength/MPa	Young's modulus/ GPa	Poisson's ratio
Mortar	2350	54.5	3.8	24	0.21
Aggregate	2557	10	1.2	5.7	0.15
Component	$f_{\text{ts-ITZ}}$/MPa	G_{I}^{C}/(N·m^{-1})	τ_{ITZ}/MPa	G_{II}^{C}/(N·m^{-1})	
ITZ	3.4	10.0	6.0	100.0	

The stress in the numerical test was obtained by dividing the contact reaction force of the loading plate by the area of the contact surface, and the nominal strain was obtained by dividing the vertical displacement by the vertical length of the specimen. A comparison of the stress-strain curves for the C40 CAC static compression test and the numerical test is shown in Fig.5. It is evident that the stress-strain curve from the numerical simulations is in good agreement with the experimental results at the peak strain, peak stress and softening stage. It is tentatively concluded that the meso-mechanical model is reliable for the analysis of the compression response of CAC material, based on which a deeper analysis of the cracking and damage process of CAC can be made.

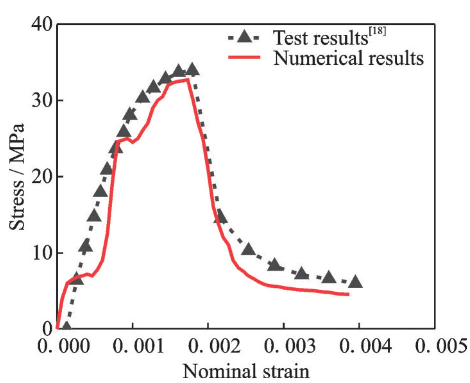

Fig.5 Comparison of stress-strain curves fornumerical and Ref.[18] tests

2.2 Analysis of cracking and damage processes

To reveal the cracking damage mechanism of CAC under static compressive loading, Figs. 6, 7 show the cracking damage process of C40 CAC with axial strain and compare it with the failure pattern of CAC in the test in Ref.[18]. A characteristic coral aggregate and its interface area with the mortar were taken from the specimen, as shown in Fig.7, and the damage process was analysed. It can be observed that due to the large strength difference between the mechanical properties of the aggregate and the mortar, and the extremely heterogeneous shape of the outer contour of the convex aggregate,

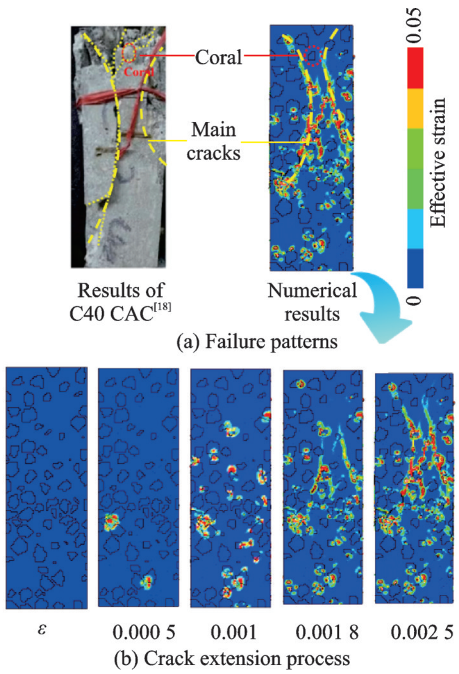

Fig.6 Comparison of numerical tests with in Ref.[18] tests

the stress concentration in the CAC occurred at the outer surface of the aggregate during the initial elastic stage. Unlike normal-strength concrete, coral aggregate has lower strength and greater brittleness than ITZ and mortar. Therefore, the micro-cracks were firstly produced at the aggregate surface, and shown in the numerical simulations as the aggregate elements failing first. But neither the ITZ elements nor the mortar elements failed, as shown in the damaging cloud for the coral aggregate and ITZ at 100 ms in Fig.7. As the load increased for 150 ms, the micro-cracks extended from the aggregate surface to the ITZ and mortar matrix in sequence. This was represented in the numerical simulation as failure fracture of the cohesive elements. At the final residual stress stage of the specimen (at 800 ms in Fig.7), the coral aggregate detached from the mortar matrix and showed surface breakage, with some cracks even penetrating the coral aggregate, which was also consistent with the description of the test results in the literature[29].

Numerous micro-cracks at the ITZ broke the bond between the coral aggregate and the cement mortar, weakening the shear resistance of the CAC and creating local oblique cracks between adjacent longitudinal micro-cracks. Further increasing the strain, the diagonal cracks developed so rapidly that

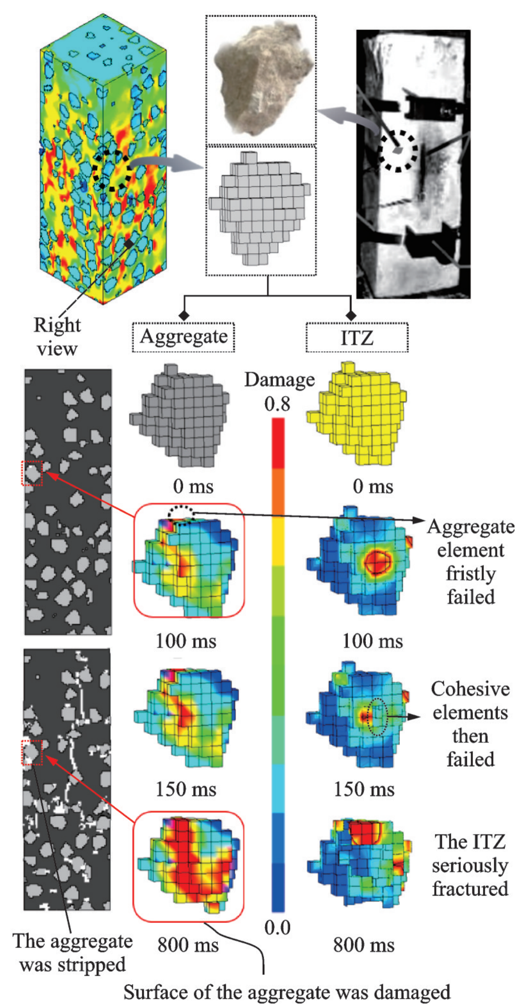

Fig.7 A characteristic coral aggregate and surface ITZ compression damage process

they penetrated the entire section to form the main diagonal cracks and extend to the concrete surface to form a macro crack zone. As can be seen from the final failure pattern of the CAC components in Fig.8, when the axial strain reached 0.35%, the angle range between the oblique crack and the vertical loading direction was 60°—75°。 This considered the angle range between the damaged surface and the loading direction. From the point of the damage distribution of each component, the damage positions of mortar, aggregate and ITZ were concentrated in the middle of the specimen along the vertical direction, where the local crack distribution was also the most concentrated. Take ITZ as an example. The failure rate of the cohesive elements in the middle of the specimen reached 54%, two to three times higher than that in the remaining positions. This is due to the large transverse frictional resis-

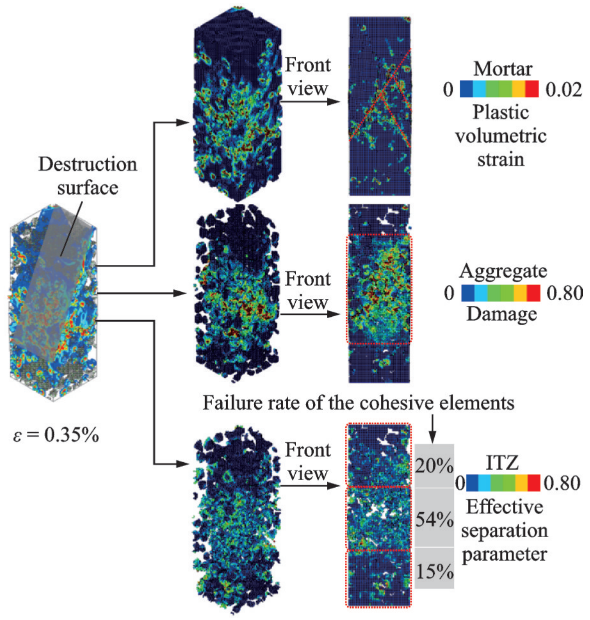

Fig.8 Final failure pattern and extent of damage to CAC components

tance at the contact surface between the loading table and the specimen, where most of the concrete elements were in a three-way compression state, with less expansion deformation and a significant increase in strength, which inhibited the expansion of cracks. Although the middle of the specimen height was close to a state of uniform uniaxial compressive stress, the expansion deformation was the largest. When the horizontal elongation strain of the specimen exceeded the ultimate tensile strain of each component of the CAC or when the concrete near the surface reached its ultimate strength under two-perimeter or three-perimeter compressive/tensile stress, it caused splitting damage, resulting in vertical cracks. This explains why most of the CAC cracks appeared on the surface and were vertically extended.

In Figs. 5, 6, the numerical simulation results were in high agreement with the test results in Ref. [18] in terms of stress-strain curves and final failure patterns, indicating that the compression properties of CAC can be well modeled using the mesoscale FDEM model developed in this paper. It also indicated that the data in Table 1 based on the theory of fracture mechanics to characterize the constitutive relationship and failure criterion of ITZ are also reasonable.

3 Conclusions

A three-phase mesoscale FDEM model was developed through C++ programming and material parameters of ITZ were introduced based on fracture mechanics theory to investigate numerically the static compressive performance of CAC. Based on the numerical and test results in Ref. [18], the main conclusions are as follows.

(1) For CAC in the initial stage of uniaxial compression loading, due to stress concentration and its weak mechanical properties, the outer contour of the aggregate will first appear micro-cracks. With the increase in loading time, the cracks will go through the ITZ and coral mortar in sequence. Finally, the cracks are mainly inclined cracks, and the angle range between the crack and the vertical loading direction is 60°—75°, which can be considered as the angle range between the damaged surface and the loading direction.

(2) According to the final failure pattern and damage distribution of each component of the CAC, the damage to the components in the central part along the vertical direction of the specimen is more severe, with ITZ showing a large amount of damage fracture, two to three times as much as the rest of the location. Some of the edges aggregates at this location show surface breakage and detach from the mortar matrix.

(3) The 3D meso-mechanical model of CAC constructed based on the FDEM is highly consistent with the experimental results in terms of stress-strain curves and final failure pattern, demonstrating that the mesoscale model and fracture mechanics model adopted in this paper can effectively describe the complex three-dimensional fracture process of CAC subjected to static compression.

In this paper, from the perspective of the macroscopic stress-strain curve and mesoscopic micro-crack propagation, the application of this meso-mechanical model to simulate the mechanical behaviour of CAC under compression-only was discussed. CAC materials are subjected to many complex stress states in practical engineering applications, resulting in different damage mechanisms and failure patterns. Therefore, the feasibility of applying this 3D meso-mechanical modeling method to CAC needs to be demonstrated in the future around a variety of load application methods.

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Author contributions Mr. **CHEN Boyu** designed the study, conducted the analysis and the results, and wrote the manuscript. Prof. **YU Hongfa** contributed to data and model components for the CAC model. Prof. **ZHANG Jinhua** complied the models and checked the manuscript. All authors commented on the manuscript draft and approved the submission.

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一种新的考虑界面特性的珊瑚骨料混凝土三维细观建模方法

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摘要:在三维随机骨料-砂浆两相细观模型的基础上,采用C++编程识别出骨料单元和砂浆单元的界面节点位置信息,在该位置处对节点离散并插设零厚度cohesive单元,之后基于断裂力学理论的裂纹能量释放率断裂准则赋予骨料-砂浆界面过渡区的失效准则,最后生成了三相有限离散元细观力学模型,成功模拟了珊瑚骨料混凝土在单轴压缩下细观裂纹扩展及宏观力学行为,表明基于该有限离散元研究方法构建的细观力学模型对模拟珊瑚粗骨料混凝土受压性能具有较好的适用性。

关键词:珊瑚粗骨料混凝土;有限离散元法;三维细观模型;断裂裂纹;C++