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Simulation Research of Self-healing Mechanism for Microcapsule Composite

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1 ABSTRACT

New composite samples，with technology of microcapsule self-healing，which are heated and compressed with matrix resin, reinforced material and fillers are prepared in this paper and three-point bending experiments are carried out. Based on the uniform materials’ crack criterion, a corresponding self-healing materials criterion is founded. Crack expanding calculation in such materials with microcapsules is made by the means of FEA software ANSYS. When cracks travel through microcapsules, stress is concentrated at the crack end and microcapsule breaks, and then the encapsulated liquid runs out to fill the crack by the capillary and polymerization with catalyst in the composite. As a result, the crack is healed. Function of self-healing is proved feasible.

2 INTRODUCTION

New composite materials which are heated and compressed with matrix resin, reinforced material and fillers have wide potential applications because they are valid dampers, fine scream absorbers and with low-pollution and expenses[1]. Under periodic heat or mechanism load, micro-cracks will be produced in matrix resin. Converge of micro-cracks will induce other breakage such as break in fibers and matrix or slippage on interfaces [2]. These damnifications are sometimes in the deep layer of structures and it is not easy to detect and repair is almost impossible.

Illuminated by organism’s self-healing up phenomenon, microcapsules filled with healing liquid are embedded in composite materials. When cracks travel through microcapsules, stress at the crack end is concentrated and microcapsule breaks, and then the encapsulated liquid runs out to fill the crack by the capillary effect and polymerizes with catalyst in the composite. As a result, the crack is healed and underlying dangerous defects are removed. Material intensity and life-span are enhanced [3].

Domestic and overseas research on the technology of self-healing microcapsules is still in the phase of exploring at present. As large amount of factors affecting healing efficiency crack criterion of microcapsule shell is discussed for one certain recipe sample based on facture theory in uniform materials. Self-healing mechanism is simulated by means of general FEA software ANSYS and self-healing function of such materials is proved feasible.

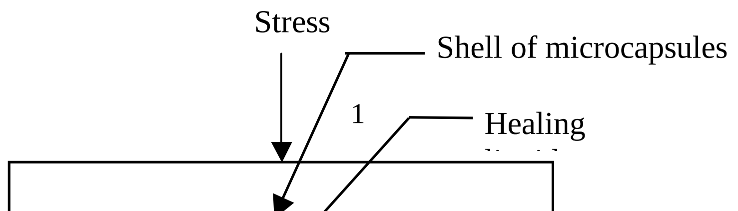


Fig. 1 Samples with microcapsules

3 EXPERIMENTS

3.1 Sample preparation

The new composite materials are mixed, heated and compressed with matrix resin, reinforced materials and fillers. Previous research [4] shows that healing efficiency reaches peak when microcapsule content is 5% of matrix. Taking integral references and previous works into considering, the detailed recipes for this paper are as follows: inorganic modified resin is applied as matrix and its weight content is 11%. Dicyclpentadiene (DCPD) microcapsules coated with epoxy resins as self-healing capsules are chosen and their weight content is 0.6%. Reinforced fiber weight content is 30%. Total weight content of various fillers is 58.4%. Samples preparation process is as follows: matrix resin, reinforced materials, fillers and microcapsules are fully mixed and enclosed into pre-heated models while pre-heating temperature is 393-433K and pressing temperature is 433-473K. Pressing stress is 13-20 MPa and heat and press preservation time is 10-15min. Then pressed roughcasts are encased into ovens and heating to 453-473K in 2-4h and maintained for 6-10h. Required standard-sized samples of 140*25*34 mm are prepared after necessary machining. Sample structures are sketched in Fig.1.

3.2 Simulation experiments

Three-point bending experiments are carried out on LDS-SOP electronic extending tester [5, 6]. Librating signals are collected and processed by Vib'SYS processor and data are analyzed with program Vl.02. Yielding and elasticity limit of unsaturated polyester resins and epoxy resins are obtained and their property parameters are shown in Tab.1. One gap is pre-cut by means of machining before bending testing. Sample fracture characters are tested by techniques of three-point bending. Samples break at load of 397 N.

Table 1. Property parameters for unsaturated polyester resins and epoxy resins

Matrix	Yielding limit σ_s / MPa	Modulusofelasticity E / GPa	Poisson's ratio ν
unsaturated polyester resins	7.37	1.438	0.35
epoxy resins	7.8	1.65	0.33

4 CRACK CRITERION ANALYSES FOR SELF-HEALING MATERIALS

4.1 Crack criterion analyses for uniform materials

Stress intensity factor K is a parameter to describe stress field degree in the zone of crack end. Crack's unstable extending depends on value of K. Thus criteria can be established according to factor K (K criteria) i.e. K=Kc. Implication of this equation is that when stress intensity factor K in the zone of crack end for an elastomer acted by outward load reaches this material's critical value Kc, the underlying crack will extend unstably and such component with crack will break. For Ⅰ-typed crack, when stress intensity factor K in the zone of crack end reaches critical value, i.e.

$$K_I = K_c \qquad (1)$$

is at critical state. Therefore brittleness fracture condition for this component with crack is：

$$K_I \geq K_c \qquad (2)$$

here Kc is regarded as fracture toughness which can be tested by related experiments. Kc has relationship with experiment temperature, thickness of tested board, rate of distortion etc.. If all the above exterior factors remain consistent, it can be regarded as a constant denoting material's natural property. Thus relationship of critical value of crack length and acting stress (or relationship of crack length and critical acting stress value) can be deduced with materials fracture toughness in brittle fracture phase. Both theoretical analyses and experiments prove that Ⅰ-typed crack is the easiest to produce brittle fracture. Meanwhile in the condition of two dimension plane strain, stress is as follows in the zone of crack end: x =y , z=(x +y). Crack is easy to expand. Consequently thick board with Ⅰ-typed crack is commonly used to test to measure critical value of stress intensity factor KIc in the condition of two dimension plane strain. That is called "fracture toughness in the condition of two dimension plane strain" for short. Curve of KIc VS thickness of tested board is shown in Fig.2.

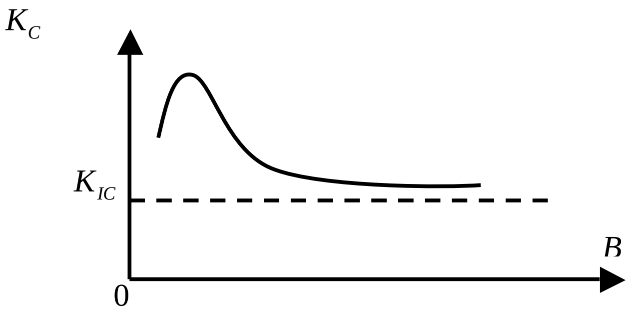


Fig. 2 Curve of KIc VS thickness of tested board

Therefore, criterion of brittle fracture for -typed crack in the condition of two dimension plane strain is:

$$K_I \geq K_{IC} \qquad (3)$$

Curve in Fig.2 indicates that KIc is the steady low value in the range of thickness above limit. Stress intensity factor Kc is the response of crack substance under exterior load. It can be calculated with theories in elasticity mechanics. While KIc is only one of the material's nature properties which reflects its brittle fracture resistance and it can be measured by experiments.

4.2 Fracture mechanical analyses for elastic flaw problems

Crack and flaw, as two typical disfigurements, commonly exist in current engineering materials [7]. Fig. 3 is the sketch of a two dimension infinitude elastic body Ω0 with one crack Γ and one round elastic flaw Ω1. Body Ω0 and flaw Ω1 are supposed to be glued together ideally in the interface L between them. Take counter-clockwise as positive. With boundary integral equation crack’s stress intensity factor can be calculated under uniform stress from infinitude end:

$$K_I(A) = -\lim_{t\to A}\sqrt{2\pi\left|t-A\right|}\cdot H(t) \qquad (4)$$

$$K_I(B) = \lim_{t\to B}\sqrt{2\pi\left|t-B\right|}\cdot H(t) \qquad (5)$$

Here $t\in\Gamma$,H(t) is the function involved in interface displacement density and plane stress. As crack is tiny, KI（A）equals to KI（B）.

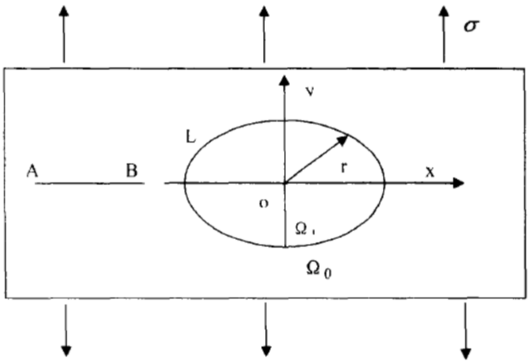


Fig.3 Infinitude elastic body with straight crack and round flaw

4.3 Fracture criterion of microcapsule shell in self-healing materials

Self-healing composite materials can be modeled as interaction of cracks and microcapsules filled with liquid [8]. Its action is more complex than solid elastic flaw. Aims of designing this new self-healing material are as follows: when the crack meets a microcapsule filled with healing liquid, its shell will break and liquid flow out to polymerize and thus cracks can be healed.

In order to obtain self-healing the material’s fracture laws, plastic stress field in the zone of crack end should be analyzed based on plastic mechanics. J integral theory is one of the requirements. Due to non-linear relations between stress and strain in plastic distortion, it is much more difficult to deal this problem mathematically. For the sake of avoiding seeking plastic stress field in the zone of crack end, J.R.Rice take it for granted that the crack end is one singularity. Eshelby’s energy and tensor integral concept is quoted and J integral theory is established by this way [9].

Rice’s J integral definition of plane crack problem is:

$$J = \int_\Gamma \left(Wdy - T_i\frac{\partial u_i}{\partial x}ds\right) \qquad (6)$$

here

$$W = W(\varepsilon_{ij}) = \int_o^{\varepsilon_{ij}} \sigma_{KI}\, d\varepsilon_{KI} \qquad (7)$$

is density of strain energy in substance with cracks (strain energy in unit volume). Ti is a facial force vector of plane unit dsdz corresponding line unit ds along loop Γ. μ i is a displacement vector. Loop Γ is a random curve starting from any point on the lower face of crack and ending at any point on the upper face of crack counter-clockwise. Besides this curve’s leading direction is supposed as the positive for arc s.

Green Formula proves that the value of J integral keeps consistent for any loop enclosing the crack end i.e. value of J integral is independent of loops. The value of J integral for Ⅰ-typed crack is expressed as JI. The critical value JIc in the condition of plane strain is measured by experiments and it is also one of the materials nature properties. Abundant research work shows that

$$J_I \le J_{IC} \qquad (8)$$

can be applied as a criterion for crack’s unstable growth.

As for the linear elastomer or in linear elastic phase, Rice proved the following relationship for Ⅰ-typed cracks firstly:

$$J_I = \frac{1-v}{E} K_I^{\,2} = G_I \quad \text{(plane strain)} \qquad (9)$$

This formula indicates J integral is equivalence to release ratio of strain GI. By this relationship JIc can be obtained indirectly by means of measure materials KIc.

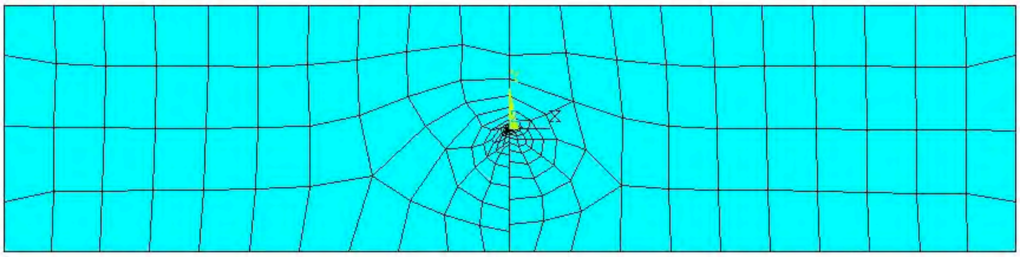
5 FEA RESEARCH OF CRACK GROWTH FOR SAMPLES WITH MICROCAPSULES

5.1 Establishment of FEA model

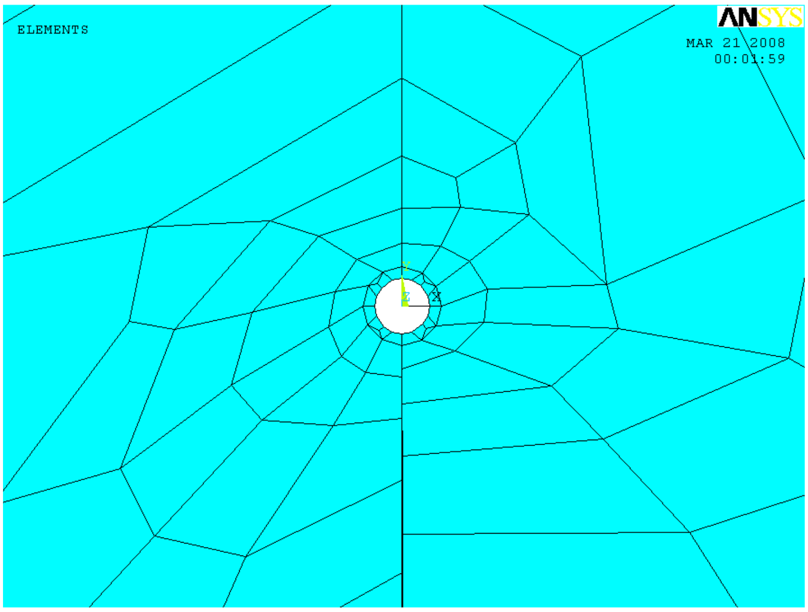
Simplifying the process is required before modeling. First of all, no account of enclosing liquid’s influences on shell materials is taken. Secondly tester’s loads on samples are simplified as concentrated force P. Thirdly based on sample’s symmetry, the central plane is chosen for calculation. In the light of elastic mechanics, the maximum concentrated stress exists on this plane. In this way the complicated three-dimension problem is simplified to two-dimensional calculation. Plane model can be established according to the size of samples.

5.2 Meshing

Cell PLANE82 in ANSYS two-dimension cell library is applied for matrix and simulated capsule materials. Because cell PLANE82 has high precision for both quadrangle and triangle blending meshes and it can accommodate abnormal shapes [10]. This 8-node cell has consistent displacement figure function and it can adapt curves boundaries well. For the sake of improving calculation precision, regular meshes are applied as much as possible avoiding mesh’s over-distortion. Model’s meshing is shown in Fig. 4(a) and the local magnifying plot is shown in Fig. 4 (b). The meshing plot shows that matrix’s grids below microcapsules become dissymmetry because of tiny crack’s location. Nodes on the lower crack plane under microcapsule are on the different positions.



（a）



（b）

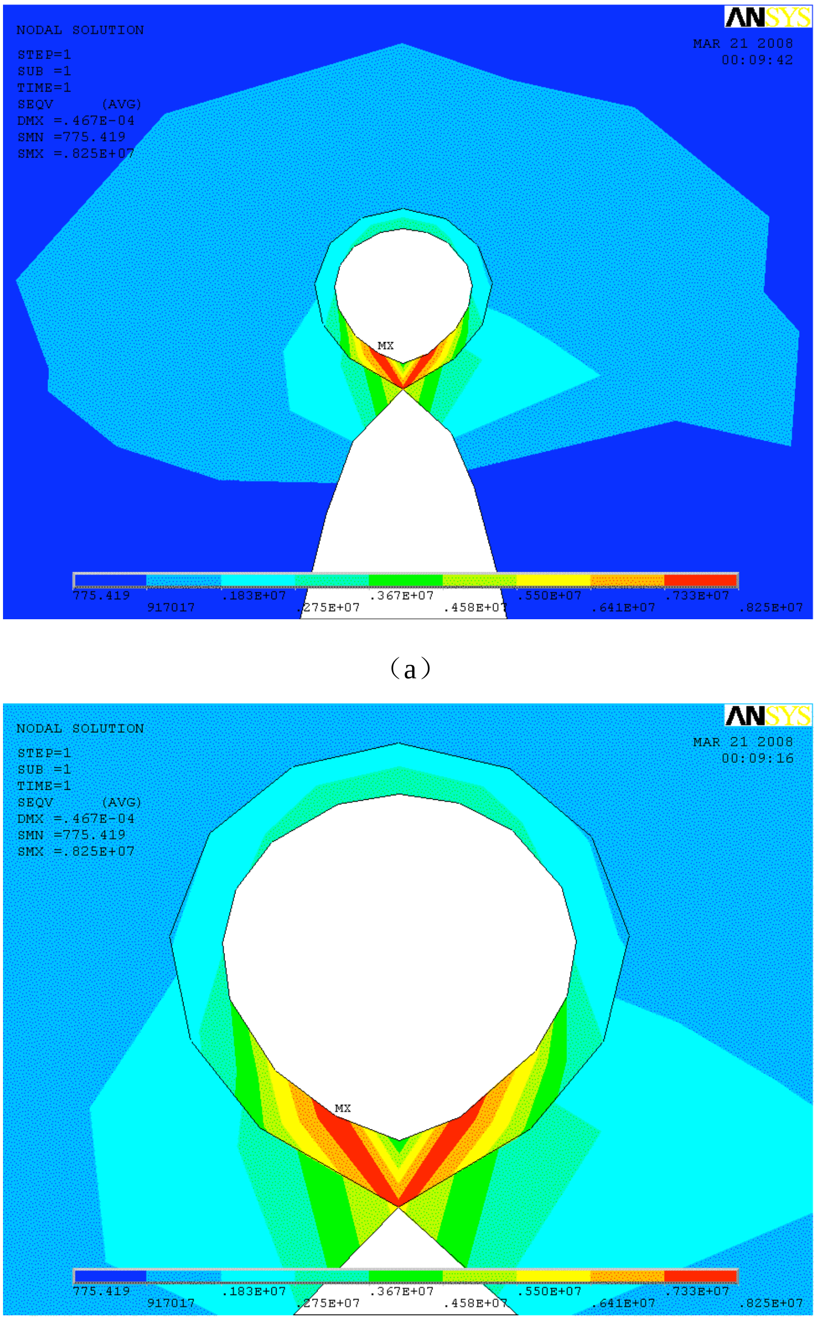
Fig. 4 Meshing plot for model sample with simulated microcapsule

5.3 Load and analysis

Fixed restriction is applied at two ends of the bottom surface to limit sample’s displacement in Y direction and movement in the direction of X is free. A concentrated load P is applied on the upper central section and calculation is processed by ANSYS.

5.4 Results and discussion

Model’s stress plot in ASYS is shown in Fig. 5. It indicates that in the zone of crack top end contacting with microcapsule there are serious stress concentrations. Crack’s stress concentration degree in microcapsule is much more serious than in matrix. Fig.5 (b) reveals zooming in stress plot neighboring microcapsule and it shows that the maximum stress appears at the contact spot of crack and microcapsule and the value of it is 8.25 MPa. It exceeds the yielding limit of epoxy resins 7.8 MPa, from which the microcapsule is made, measured in section 2.2 and microcapsule will fracture definitely. Maximum concentrated stress in matrix appears below microcapsule and its value is 6.2 MPa approximately which is below the yielding limit of unsaturated polyester resins 7.37 MPa measured in section 2.2. Therefore matrix material is safe.



（a）

（b）

Fig. 5 Stress plot of model sample with simulated microcapsule

The above calculation results indicate that during the crack growth phase, the maximum concentrated stress in microcapsule exceeds its yielding limit while that value in matrix is below the corresponding yielding limit. Hereby crack will travel through the microcapsule definitely and arouse self-healing function in this composite material. The calculation results approves that microcapsule self-healing technology is feasible from the point of theory.

6 CONCLUSIONS

(1) Yielding limits of unsaturated polyester resins and epoxy resins, materials for matrix and microcapsule, are measured by means of three-point bending experiments;

(2) Fracture criterion of microcapsule shell in self-healing materials is established by theoretical inductions;

(3) FEA calculation with ANSYS approves microcapsule self-healing technology is feasible from the point of theory.

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