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Progressive damage modeling of porous composite materials by multi-scale finite element method

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Abstract

Porous composite materials have a wide spectrum of applications in the aerospace and marine industries and biomedical engineering. A multi-scale finite element method (FEM) incorporating the element-failure method (EFM) and the strain invariant failure theory (SIFT) was proposed to simulate the progressive damage of porous composite materials under compression in this study. In micro-scale, a three-dimensional FE repeated cell model was constructed to determine the mechanical properties of the base composite material. Moreover, two-dimensional porous repeated cell models in macro-scale were developed to predict damage propagation in the porous polymer composite. The porous models with three different arrays of pores were constructed to investigate the effect of spatial arrangement of the pores on the progressive damage behavior of the porous composites. Porous hydroxyapatite/ polyetheretherketone (HA/PEEK) composites under compression loading was chosen as a case example to illustrate the implementation of the proposed method. The simulation results showed that the proposed method was feasible and effective in simulating the progressive damage behavior of porous composite materials. The model with the hexagonal arrangement of pores was found to be more resistant to damage propagation under compression loading.

Key words: Multi-scale, Porous composite materials, Element-failure method, Strain invariant failure theory, Progressive damage, Finite element method

1. Introduction

Over the past few decades, polymers have been widely used to replace many of the conventional metals in various engineering and medical applications, because polymers possess some distinctive advantages such as ease of processing, lighter weight and lower cost. However, the stiffness of polymers cannot generally satisfy the engineering requirement for load-bearing applications (Kurtz et al. 2007) . As the stiffness and strength of polymer can be improved with addition of fillers such as fibers and particulates, the mechanical properties of the particulate polymer composites have been extensively studied in past decades (Cogswell et al. 1992, Tsui et al. 2004, Ichim et al. 2007). Various finite element (FE) models have been developed to study the effects of the fillers on the properties of various composites, so as to control the size, shape, amount and distribution of the fillers. Damage is one of the most important factors causing the failure of polymer biomaterials, especially under excessive loading (Ichim et al. 2007, Wiggins et al. 2003). Recently, particle-matrix debonding and micro-damage of the base material and interphase layer have attracted attention of many researchers (Wiggins et al. 2003, Tsui et al. 2001, Fan et al. 2004) for better prediction of the mechanical properties of polymer composites.

At present, synthetic polymer based porous structures have shown promising performance in aerospace, marine, and biomedical applications due to many practical advantages arising from precise control of material composition, porosity, and micro- and macro-structural properties. Rezwan et al. have reviewed various techniques for producing porous polymer-ceramic composite structures of different morphologies, whose properties depend on not only the size and shape of the particle, but also arrangement of voids and porosity. Load-bearing capability of these structures could be significantly weakened by high porosity. Failure often occurs when the strength of the structural material cannot support the applied loading. Therefore, the design and fabrication of porous composite materials especially made of polymers with adequate load-bearing capability become an important research topic.

A scalar damage variable is often defined for depicting the degradation behavior of materials. For the conventional stiffness reduction approach, the values of certain material parameters in the constitutive equations will be reduced when damage occurs. However, the stiffness matrix of the FE model may become ill-conditioned, leading to divergence or instability in computation. For another approach called the element failure method (EFM) (Beissel et al. 1998), only the nodal forces of damaged elements are modified in the EFM. Therefore, the stiffness matrix remains unchanged in the whole simulation process, so that the aforesaid computation problem can be avoided. So far, the EFM and the SIFT (Gosse et al. 2001) have been applied for predicting damage, fracture, and delamination of composites (Tay et al. 2006, Tay et al. 2006, Tay et al. 2008). To the best of authors' knowledge, their application in porous polymer composites has not been discussed in open literatures.

The purpose of the present work was to develop a multi-scale FE method for investigating the effect of spatial arrangement of pores on the progressive damage behavior. By using the EFM and the SIFT, a damage model was developed to bridge the gap between the microscopic damage phenomenon and the macroscopic mechanical behavior. The effects of three different pore arrangements in the porous composite material were analyzed and compared, and thus the optimal design was discussed on a scientific basis.

2. Material and methods

2.1 Choice of Material

Porous hydroxyapatite/polyetheretherketone (HA/PEEK) polymer composite materials have been used as a potential biomaterial for bone replacements and tissue engineering applications [10], and was used as the target material in the present work. HA is a bioactive material with the calcium-to-phosphorus ratio similar to that in natural bone. PEEK is a rigid semi-crystalline polymer which has superior mechanical properties and bone-like stiffness as well as many other benefits, such as good resistance to chemical, fatigue, wear and high temperature. The mechanical and biological properties of HA/PEEK porous composite can be controlled by a number of factors such as the pore architecture, porosity level, damage behavior of the constituent materials, and interfacial property between the matrix and the particle.

2.2 Multi-scale FE modeling process

2.2.1 Micro-scale FE modeling

A three-dimensional (3D) micro-scale FE model (Fan et al. 2004) was constructed for predicting the mechanical behaviors of the base composite material, HA/PEEK. The FE model consisted of three different phases: a spherical HA particle, PEEK matrix, and the interfacial layer between the particle and the polymer matrix as shown in Fig.1(a). As reinforcing particles were assumed to be evenly distributed in the polymer matrix, a periodically repeated cubic array was employed to be the representative volume element (RVE) of the base material. Due to the symmetry for the packing of the spherical particles, only one-eighth of the repeated micro-cell as shown in Fig.1(a) was considered in the computation. The particle volume fraction (PVF) V_p is given by

$$V_p = \frac{4\pi}{3}\left(\frac{r_1}{r}\right)^3 \tag{1}$$

where r_1 is the radius of spherical particle, and r is the length of the micro-cell.

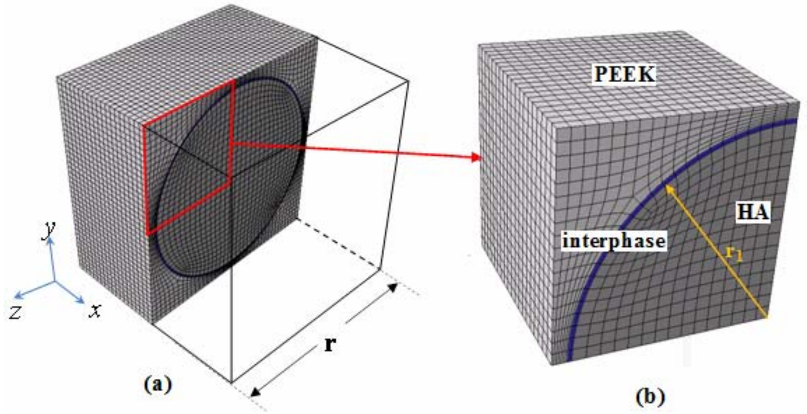


Fig. 1. Micro-scale cell model (a) RVE; (b) 1/8 RVE.

The thickness of the interphase layer was set to be 1% of the micro-cell length (Fan et al. 2004, Wu et al. 2002). The bonding among the particle, the matrix and the interfacial layer was assumed to be initially perfect. According to the study of Wu et al. 1995, Young's modulus of the interfacial layer was given to be one-twentieth of that of PEEK and the Poisson's ratio was set to 0.48. The mechanical properties of the constituent materials adopted in the FE computation are summarized in Table 1 (Fan et al 2004, Wu et al. 1995).

Materials	E(GPa)	ν	p(kg/m^3)
PEEK	3.2	0.42	1291
HA	85	0.3	3160
Interfacial layer	0.16	0.48	N/A

Table 1. Mechanical properties of the constituent materials.

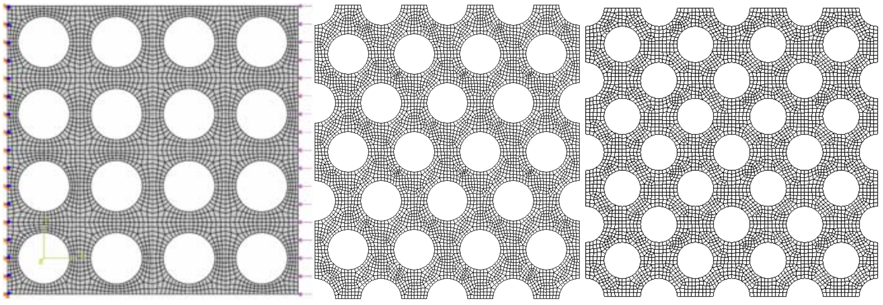
Due to the symmetry of the unit cell model as shown in Fig.1(b), the normal displacements (u, v, w) on the symmetrical surface in the (x, y, z) directions were constrained such that

$$\begin{aligned} u &= 0 \text{ on } x = 0, \\ v &= 0 \text{ on } y = 0, \\ w &= 0 \text{ on } z = 0. \end{aligned} \tag{2}$$

Moreover, the symmetrical surfaces of the cell model were maintained to remain plane and parallel to their initial state after deformation, in order to ensure compatibility among all periodic representative cells.

2.2.2 Macro-scale FE modeling

In macro-scale, a porous composite material made of HA/PEEK under compression was studied. In general, the mechanical properties of porous composite material depend directly on the shape and spatial distribution of the pores. Three different spatial pore arrangements (Tay et al. 2008), namely, square, hexagonal and diamond, as shown in Figs.2(a)-(c), were employed in modeling the porous HA/PEEK composite. Two-dimensional plane strain macro-models were constructed to simulate the progressive damage process in the entire porous structure. Due to the symmetry of structural and loading property, a quarter of the entire porous structure was modeled (Fig.2).



a) (b) (c)

Fig. 2. Macro-scale FE models under three spatial arrangements of pores, (a) square, (b) hexagonal, and (c) diamond.

For computation in the macro-scale, the mechanical properties of the base composite material were represented mathematically by the Halpin-Tsai equations (Wu et al. 2002). The apparent Young's modulus and Poisson's ratio of the composite material are respectively given by

$$\begin{aligned} E &= E_m\left(\frac{1+\zeta\eta f}{1-\eta f}\right) \\ v &= f v_f + (1-f)v_m \end{aligned} \tag{3}$$

where E_m and E_f are Young's moduli of the matrix and the particle, respectively. v_m and v_f are the Poisson's ratio of the matrix and the particle, respectively. f is the value of PVF. The parameter η is given by

$$\eta = \frac{(E_f/E_m)-1}{(E_f/E_m)+\zeta} \tag{4}$$

where the factor ζ was used to describe the influence of filler geometry on a particular property. For the spherical particles, ζ is in the following form,

$$\zeta = 2 + 40f^{10} \tag{5}$$

For the three macro-models, the porosity was set to 0.4. The Young's modulus and Poisson's radio of the porous composite calculated from Eqs.(3)~(5) were equal to 8.6GPa and 0.37, respectively. In this simulation, the sizes of the HA particle and the pore were assumed to be in order of 10μm and 1mm, respectively, for satisfying the dimensional requirement of RVE. The left line of all macro- models shown in Fig.2 were both constrained in the x and y directions, while the right line was subjected to a controllable compression loading. The loading and boundary conditions in the three different spatial arrangements of pores are identical for comparison. The complete simulation was executed on an Intel Core i5/2.67GB computer with 4GB RAM.

2.3 Progressive damage modeling

The SIFT proposed by Gosse et al. 2001 was used as the damage criterion of polymer composites by amplifying the strain invariant quantities through extracting the information from the micro-scale FE models (Tay et al. 2005, Tay et al. 2008). According to the SIFT, there are three strain invariants. The first, second and third invariants, J_1, J_2 and J_3 were defined as

$$J_1 = \varepsilon_x + \varepsilon_y + \varepsilon_Z \tag{6}$$

$$J_2' = \frac{1}{6}[(\varepsilon_x - \varepsilon_y)^2 + (\varepsilon_y - \varepsilon_Z)^2 + (\varepsilon_Z - \varepsilon_x)^2] - \frac{1}{4}(\varepsilon_{xy}^2 + \varepsilon_{yz}^2 + \varepsilon_{xz}^2) \tag{7}$$

$$J_3 = \varepsilon_{vm} = \sqrt{3J_2'} \tag{8}$$

Thirteen typical locations on the micro-cell model as shown in Fig.3 were chosen for extraction of the local strain amplification factors (SAFs). Points P1~ P4, I1~ I3 and M1 to M6 were located at the reinforcing particle, the interfacial layer, and the polymer matrix, respectively. The extraction method of SAF proposed by Buchanan et al. 2009 was used. For a prescribed point k^{th} within the RVE, the strain, ε_i^k was obtained from the following equation:

$$\varepsilon_i^k = M_{ij}^k \bar{\varepsilon}_j, (i, j = 1 \cdots 6) \tag{9}$$

where M_{ij}^{k} is the strain amplification factor matrix and $\bar{\varepsilon}_j$ is the arbitrary state of strain applied to the RVE.

The components of the SAF matrix were determined uniquely by prescribing a canonical state of deformation and carrying out 3D FE analyses. For example, it was assumed that $\bar{\varepsilon}_j = 0, (j = 2 \cdots 6)$ and $\bar{\varepsilon}_1 = 1$, then the strain, ε_i^k becomes,

$$\begin{aligned} &\varepsilon_1^k = M_{11}^k \bar{\varepsilon}_1, \text{ or } M_{11}^k = \varepsilon_1^k;\ \varepsilon_2^k = M_{21}^k \bar{\varepsilon}_1, \text{ or } M_{21}^k = \varepsilon_2^k \\ &\varepsilon_3^k = M_{31}^k \bar{\varepsilon}_1, \text{ or } M_{31}^k = \varepsilon_3^k;\ \varepsilon_4^k = M_{41}^k \bar{\varepsilon}_1, \text{ or } M_{41}^k = \varepsilon_4^k \\ &\varepsilon_5^k = M_{51}^k \bar{\varepsilon}_1, \text{ or } M_{51}^k = \varepsilon_5^k;\ \varepsilon_6^k = M_{61}^k \bar{\varepsilon}_1, \text{ or } M_{61}^k = \varepsilon_6^k \end{aligned} \tag{10}$$

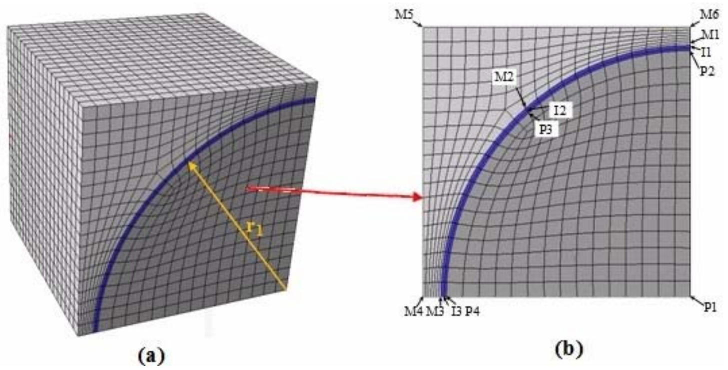


Fig. 3. 1/8 of RVE; (b) 13 typical positions for the extraction of SAF from the micro-scale model.

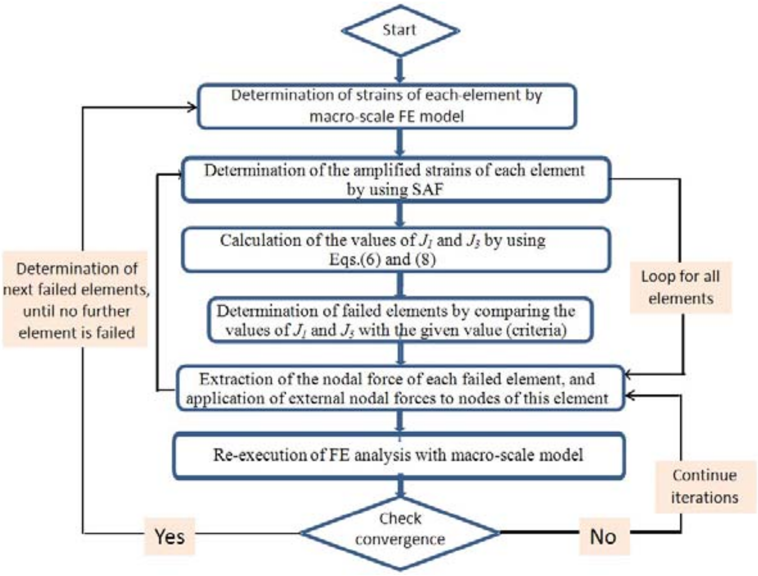


Fig. 4. A flowchart for implementation of the progressive damage simulation.

Figure 4 shows the flowchart for executing a simulation for the progressive damage process of the porous polymer composite material under compressive loading. The whole simulation process was realized using the commercial FE software named ABAQUS, while the EFM and the SIFT were incorporated into ABAQUS by writing a user-defined subprograms with Python based on ABAQUS Scripting Interface (ASI). Strains of each element were determined by multiplying the strains computed from the macro-scale FE model with the SAF. The values of J_1 and J_3 were then calculated by Eqs.(6) and (8) based on the thirteen typical positions as shown in Fig.3. Once the criteria for J_1 and J_3 were met, the nodal forces of each failed element were extracted and external nodal forces would be applied to these nodes, while the material stiffness was kept unchanged. The steps for extracting nodal forces of failed element and their application as external forces to the nodes followed those reported by Tay et al 2008. Finally, the FE analysis of the macro-scale model would be re-executed. When a convergence was obtained, the whole program would be repeated to determine the next failed elements until no further failed elements could be found.

3. Results and discussion

Figure 5 shows the progressive damage contours for the macro-scale model with the hexagonal arrangement of pores under compression loading, in which the elements with color denotes the failed elements. It can be seen that the porous polymer composite is gradually degenerated with increasing compression loading, because of increasing number of the failed elements. Moreover, it can also be observed that the damage is initiated at the vertical poles of the pores and then propagates progressively along the loading direction. The results demonstrate that the multi-scale modeling method is feasible for simulating the progressive damage of the porous polymer composite.

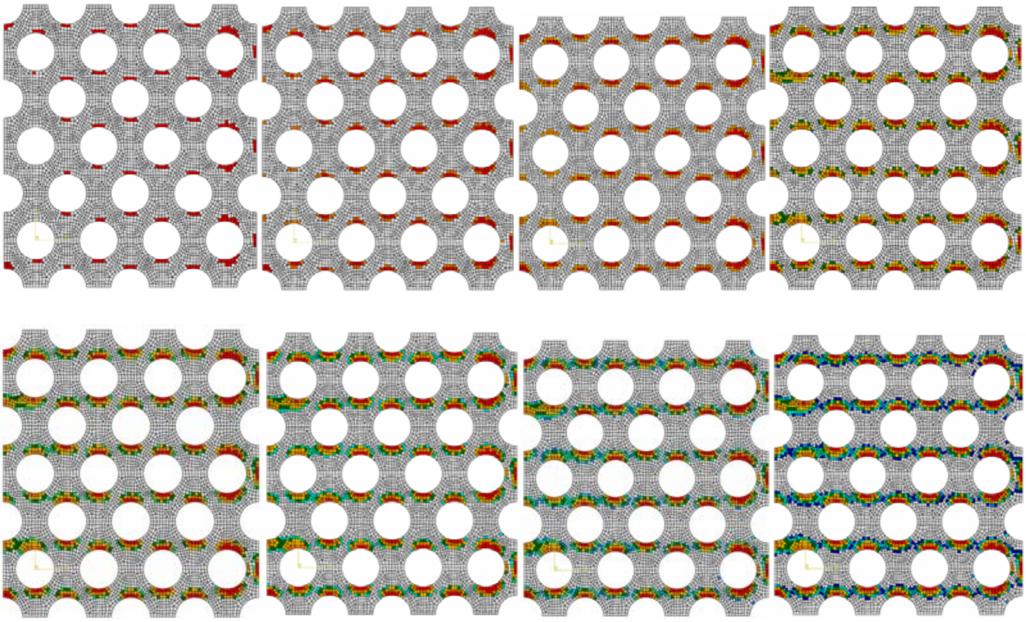
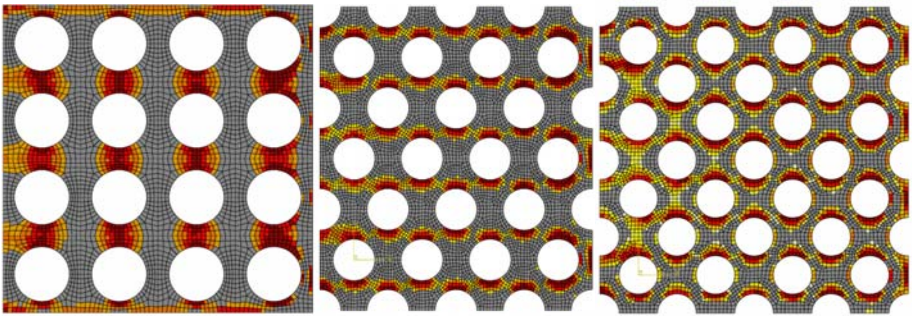


Fig. 5. The progressive damage process of the macro-scale model with the hexagonal arrangement of pores under compression loading (the damage progression starts from the upper left to upper right, and then from the lower right to lower left).

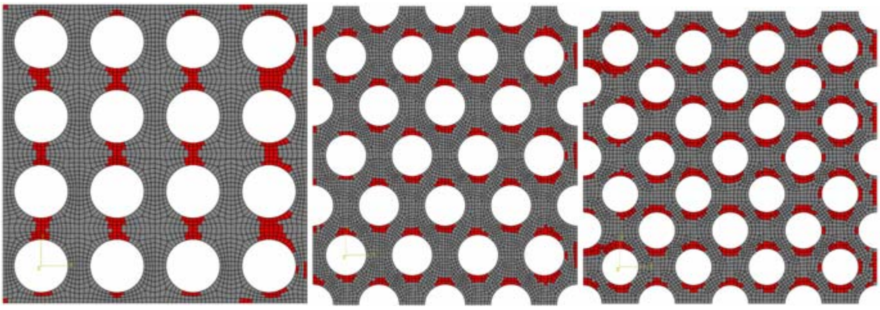
Figure 6 illustrates the damage contours of the porous polymer composites with three different spatial pore arrangements under compression. It can be observed that the damage propagation pattern is different in each case. For the hexagonal pore array, the damage propagates along the loading direction. For the square pore array, the damage propagates along the vertical direction. For the diamond pore array, the damage propagates along an angle of ±45 degree with the loading direction.



a) b) c)

Fig. 6. Predicted damage contours of the three macro-scale models with different spatial arrangement of pores under compression loading, (a) Square, (b) hexagonal, and (c) diamond.

Figure 7 shows the progressive damage contours for three different cases under the same compressive displacement of 5mm. It can be observed that the model with the square pore array was not the worst one in terms of the capacity of resisting damage, because the damage was already localized across the regions connecting the pores along the vertical direction. On the other hand, the number of failed elements at the vertical poles of the pores in the model with the hexagonal pore array was less than those in the model with the diamond pore array, indicating that the model with the hexagonal pore array has the better capacity of resisting damage.



a) b) c)

Fig. 7. Predicted damage contours of the three macro-scale models with different spatial arrangement of pores under the same compressive displacement of 5mm, (a) Square, (b) hexagonal, and (c) diamond.

4. Conclusion

The multi-scale FE modeling approach incorporating the EFM and the SIFT has been successfully developed to simulate the progressive damage processes of porous HA/PEEK polymer composites. This approach has shown to be effective in establishing damage criteria to identify the failed elements and enable the prediction for the progressive damage processes of the composites. The effects of three different pore arrangements on the porous composites could also be simulated so as to determine the preferred spatial arrangement of the pores. The model with the hexagonal array of pores has been found to possess higher capacity of resisting damage.

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Извод

Моделирање ширења оштећења прозних композитних материјала помоћу мулти-скалне методе коначних елемената

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Резиме

Порозни композинтни материјали имају широк спекар примена у ваздухопловству и поморској индустрији и биомедицинском инжењерингу. У овом раду је предложена вишескална метода коначних елемената (ФЕМ) која обухвата методу отказа елемента (ЕФМ) и теорију отказа засновану на инваријантама деформација (СИФТ), за симулацију ширења оштећења порозних композинтних материјала услед компресије. На микро-нивоу, конструисан је тродимензонални ФЕ модел са понављањем ћелија како би се одредила механичка својства основног композинтног материјала. Поврх тога, дводимензоналнки модел порозне ћелије са понављањем на макро нивоу је развијен како би се предвидела простирање оштећења у порозном полимерном композиту. Порозни модели са три различита реда пора су конструисани за испитивање ефекта просторне расподеле пора на понашање прогресивно оштећење порозних композита. Порозни "худрохуапатите/ полуетхеретхеркетоне (ХА/ПЕЕК)" композит под копресионим оптерећењем је изабран као пример илустрације примене предложене методе. Резултати симулације показали су да је предложена метода била изводљива и ефикасна за симулацију понашања прогресивног оштећења порозних композитних материјала, Модел са хексагоналним распоредом пора се показао као отпорнији на ширење оштећења услед оптерећења на компесију.

Кључне речи: Мулти-скални, порозни композинтни материјали, метода отказа елемената, Теорија заснована на инваријантама деформација, прогресивно оштећење, метода коначних елемената

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