

Mechanical behavior of composite gel periodic structures with the pattern transformation

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ABSTRACT

When the periodic cellular structure is loaded or swelling beyond the critical value, the structure may undergo a pattern transformation owing to the local elastic instabilities, thus leading to structure collapses and the change to a new configuration. Based on this deformation-triggered pattern, we have developed the novel composite gel material. This designed material is a type of architecture material which achieves special mechanical properties. In this paper, the mechanical behavior of the composite gel periodic structure with pattern transformation has been studied through numerical simulations. When pattern transformation occurs, it can result in a different elastic relationship compared with the material at untransformed state. From the obtained nominal stress versus nominal strain behavior, the Poisson's ratio and corresponding deformed structure patterns, we investigate the effects of the uniformly distributed gel inclusions on composite material, thereby having a better understanding of the characteristics of composite materials. We hope this study can provide future perspectives for the new composite material.

1. INTRODUCTION

Periodic cellular structure has been widely investigated for generating novel pattern transformation and special mechanical properties. When it is loaded or swelling beyond the critical value, this type of periodic structure can exhibit structural instabilities (Mullin et al., 2007), thus leading to structure collapses and the change to a new configuration. The structure with the new configuration can display a special mechanical property. It is imperative to study the influence of instabilities on global material properties. Thus the researchers can design the structure of the material to achieve or expand the special functionality of material. Evans and Alderson had modeled chiral and anti-chiral honeycomb material structures, and considered the deformation mechanisms responsible for auxetic functionality of the two structures (Alderson et al., 2010). Besides the honeycomb structures, the other shapes

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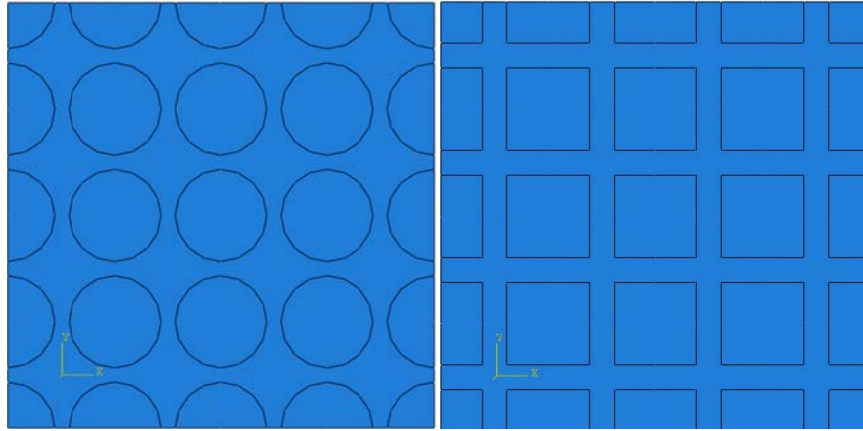
of re-entrant structures (Barnes et al., 2012; Gaspar et al., 2011; Miller et al., 2011) or buckliball (Shim et al., 2012) have also attracted large numbers of researchers to study the pattern transformation of those structural materials, especially for studying the critical value of applied load for different pattern. Meanwhile, Mullin group has studied mechanical properties of the porous elastic material structures through theory, simulations and experiments (Bertoldi et al., 2008; Bertoldi et al., 2010; Mullin et al., 2007; Willshaw and Mullin, 2012). In the application of structural materials, Jang et al. (2009) and Li et al. (2012) combined pattern instability and shape-memory hysteresis for photonic switching. In soft structural materials, many studies of the collapse of a void or hole in an elastomer under swelling and de-swelling were carried out (Cai et al., 2010; Ding et al., 2013; Hong et al., 2009). The similar novel composite material is experimentally studied by combining the silicone rubber samples with jelly filling each of the holes (Mullin et al., 2013). From previous studies, pattern transformation is a result of a local buckling instability in the compressively loaded vertical inter-hole ligaments in the case of the arrays. Based on this novel deformation-triggered pattern, we have developed the novel composite gel structure material, in which the arrays of quadrate and circular gel particles or rods are filled into the periodic cellular structures. This designed material is a type of architecture material which can achieve special mechanical properties and display a new mechanical behavior.

In this paper, the mechanical behavior of the composite gel periodic structure with pattern transformation has been studied through numerical simulations. From the obtained nominal stress versus nominal strain curves and corresponding deformed structure patterns, the effects of uniformly distributed gel inclusions on mechanical properties of composite materials are discussed. The study can provide a better understanding of the characteristics of the novel composite gel materials.

2. MODELING OF THE COMPOSITE MATERIAL

The composite soft material that is composed of two components has already been manufactured by Mullin et al. (2013). In their experiment, the square arrays of holes in silicone rubber sheet are filled with jelly. According to the previous study, we understand that if the holes are filled with a more rigid material than that of the matrix, the cellular structure will not lead to any pattern switch (Michel et al., 2007). Therefore, a much softer material needs to be placed in the holes to achieve pattern switch for composite material. Mullin et al. (2013) has discovered that the inclusion I which has a Young's modulus of $\leq 1\%$ of the bulk does not suppress the pattern switch. Based on the Liu's work on the incremental modulus of gel (Liu et al., 2011), we try to plug the gel materials into the porous elastomers and find whether the periodic composite material can still undergo the pattern transformation, and how the gel material affects on the critical strain. In the study, the numerical simulations of composite material under compressed load are carried out to study the deformation behavior of the structure material. In the modeling, the specific combinations of two materials are modeled as illustrated in Fig. 1(a and b). The size of Fig. 1(a) is $39.88 \text{ mm} \times 39.88 \text{ mm}$, comprising a microstructure of a $9.97 \times 9.97 \text{ mm}^2$ square arrays of circular gel inclusions of 8.67 mm diameter with 9.97 mm center-to-center spacing in vertically and horizontally; The size of model in Fig. 1(b) is $40 \text{ mm} \times 40 \text{ mm}$ with $10 \times 10 \text{ mm}^2$ square arrays of 7.7 mm length

of square gel with 10mm center-to-center spacing. The volume fraction of gel in the two types of composite materials is same value of 0.59.



(a) (b)

Fig.1 Composite material structures with arrays of gel inclusions:(a) circular gel shape, and (b) square gel shape. The gel fraction in two models is the same.

2.1 Material properties

In the composite gel structural material, two different materials are used to form the composite material, i.e. PMMA (polymethyl methacrylate) for matrix and hydrogel for inclusion. For matrix material, a compressible neo-Hookean model (Michel et al., 2007) is assumed. The strain energy $W(F)$ form for neo-Hookean material in plane strain is:

$$W = \frac{\mu}{2} [(I - 2) - 2 \ln J] + \frac{\kappa - \mu}{2} (J - 1)^2, \quad (1)$$

where μ and κ are, respectively the shear and bulk moduli of the solid at zero strain. The material PMMA (polymethyl methacrylate) was modeled as nearly incompressible, characterized by $\kappa/\mu = 50$. From the early studies (Bertoldi et al., 2008; Mullin et al., 2007; Willshaw and Mullin, 2012), the initial Young's modulus was given as 3.25 MPa, so that $\mu = 0.55 \text{ MPa}$.

The inclusion material is gel material (Hong et al., 2009), with a strain energy $W(F)$ given by

$$W = \frac{1}{2} N \nu (I - 3 - 2 \ln J) - \frac{kT}{\nu} \left[(J - 1) \ln \frac{J}{J - 1} + \frac{\chi}{J} \right], \quad (2)$$

where $kT = 4 \times 10^{-21} \text{ J}$ at room temperature. The two dimensionless material parameter $N\nu$ and χ are chosen appropriately in the numerical examples below. We take the values $N\nu = 10^{-2}$ and $\chi = 0.1$.

2.2. Boundary condition

It is realized that the results of finite-sized models are necessarily influenced by boundary conditions at both loaded and traction free edges. To eliminate the boundary condition effects, the composite material can be represented as a periodic array of

representative volume elements (RVEs). Thus the numerical investigations are performed on periodic structures. Actually compared with analysis of the full finite structure model, the RVEs results exhibit an earlier switch (Mullin et al., 2007), i.e. boundary effects delay the structure transformation. Therefore, periodic boundary conditions are imposed on all cell boundaries, and the general form of periodic boundary condition can be expressed as (Berger et al., 2005; Xia et al., 2003).

$$u_i = \bar{S}_{ij} x_j + u_i^* \quad (3)$$

where \bar{S}_{ij} are the average strain, u_i^* is the periodic part of the displacement components (local fluctuation) on the boundary surfaces, which is dependent on the applied global loads. The indices i and j denote the two-dimensional coordinate directions in the range from 1 to 2.

3. PATTERN SWITCHING IN COMPOSITE MATERIAL

When periodic elastomeric cellular solid is compressed, the array of pores undergoes an unstable transformation at a critical point (Bertoldi and Boyce, 2008; Bertoldi and Boyce, 2007; Bertoldi et al., 2008; Bertoldi and Gei, 2011; Bertoldi et al., 2010; Jang et al., 2009; Kang et al., 2013; Mullin et al., 2007; Singamaneni et al., 2009a; Singamaneni et al., 2009b). Similar instabilities also trigger the change to the new configuration in the novel composite gel material. The numerical approach captures the mechanical behavior of composite material for exploring the effect of gel material and gel shape.

3.1 Stress versus strain behavior

To obtain the nominal stress vs. nominal strain response, the total force on bottom edge as shown in Fig.1 is monitored as a function of the applied displacement. The numerical results for the nominal stress versus nominal strain behavior of the two types of composite materials are shown in Fig.2. Figure 2 also provides a directive comparison between the matrix material without gel inside and the one with gel. The behavior of the composite material is characterized by an initial almost linear elastic behavior with a sudden change to a different elastic relationship. The transition point response to the pattern transformation in the composite materials and the patterns at the nominal strain of 0.2 are shown in Fig.3. At the turning point to the new configuration, much of the macroscopic deformation is observed to be accommodated by the rotation of the four matrix domains diagonally bridging neighboring inclusions; these domains experience negligible strain but undergo large rotations. Then after transformation, due to that gel inclusion suppress the motivation of the matrix domains, the rotation leads to a different composite structure from the initial state. The circular gel inclusions of the novel composite material break their initial shapes and bifurcate into ellipses of vertical and horizontal directions alternatively. Meanwhile, the linear structure of the composite matrix material with square gel inclusions changes into sinusoidal shape in the vertical direction. In addition, the pattern transformation occurs much later in the composite material with the square gel inside than the circular gel inside, though both having the same value of gel fraction.

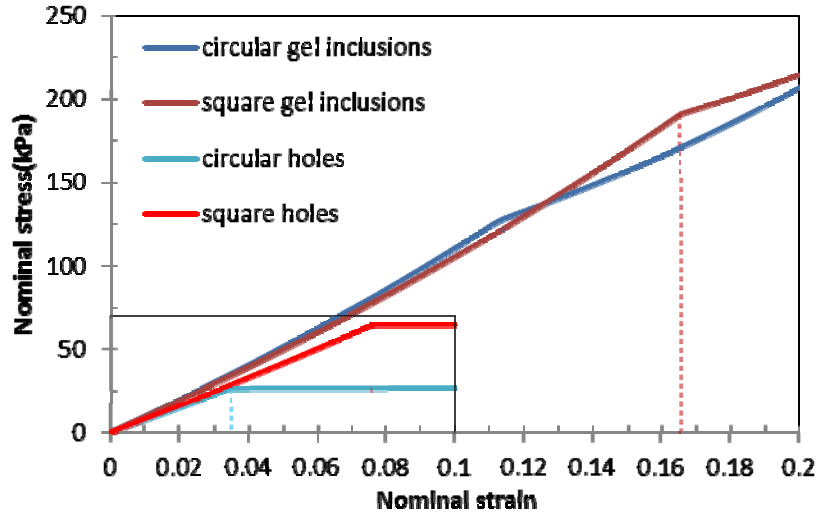


Fig.2 The nominal stress versus nominal strain behavior of the two types of structures with gel inclusions and no gel inside (The red lines represent the square holes or gel inclusions and the blue lines represent the circular holes or gel inclusions).

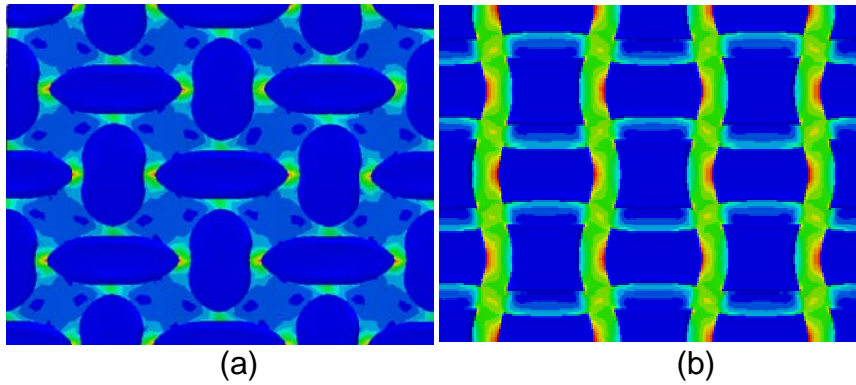


Fig.3 The new composite material structure at the nominal strain of 0.2.

Besides the different shapes of gel inclusions, the property of gel inclusion also affects the properties of the composite material. As discussed in Section 2.2, we use gel mono-phase theory to simulate the gel inclusions. The initial state of gel inclusions in these novel composite materials is characterized by the free-swelling stretch λ_0 , which is equilibrated in a solvent of chemical potential μ as follows (Hong et al., 2009),

$$N_V \left(\frac{1}{\lambda_0} - \frac{1}{\lambda_0^3} \right) + \log \left(1 - \frac{1}{\lambda_0^3} \right) + \frac{1}{\lambda_0^3} + \frac{\chi}{\lambda_0^6} = \frac{\mu_0}{kT}. \quad (4)$$

When the composite material is compressed, gel inclusions are subjected to constraint de-swelling, which is similar to the example case of a 1-D rod of a gel equilibrated in a solvent of chemical potential μ , and subjected to a uniaxial stress s_1 along the longitudinal direction. From the theoretical calculation of Liu et al. (2011), the reduced incremental modulus or tangent stiffness of gel is a function of current deformation and stretch (current chemical potential), as is illustrated in Fig. 4. According to the definition of incremental modulus of hydrogel (Liu et al., 2011), the free-swelling

states or the initial states are hence at the intersection points of the curves for different chemical potentials, which means that the modulus of gel at free swelling state is almost same. The value of the incremental modulus of gel increases as the stretch value decreases or the initial chemical potential increases.

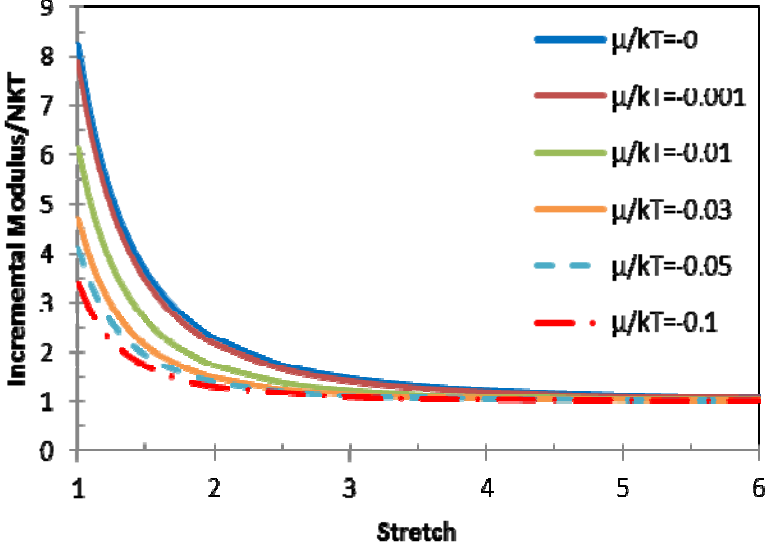


Fig.4 Incremental modulus of gel varying with stretch for various initial chemical potentials.

Now we exploit gel at free-swelling state subjected to different chemical potential, to fill the holes of porous elastic material to develop this novel composite material. Fig.5 shows stress versus strain behavior using the RVE model with array of square gel inclusions in an elastomeric matrix various for initial chemical potentials.

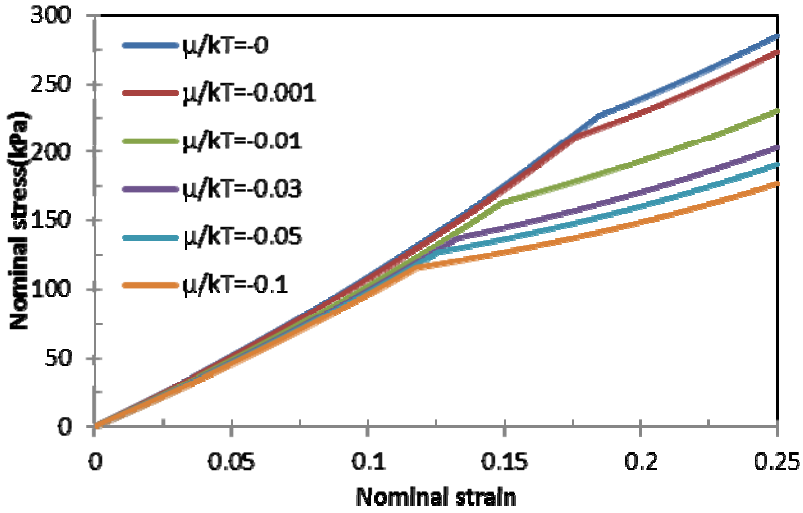


Fig.5 Stress vs. strain behaviors using the RVE model with array of square gel inclusions in an elastomeric matrix various for initial chemical potentials.

From the plots, we find out several interesting properties of the new material. Firstly, instead of perfectly linear elastic before the pattern switching, the material shows the increasing modulus because the gel inclusions becomes harder as the water in gel inclusions comes out with the applied load; so does the material after transformation. Secondly, the larger the initial chemical potential is, the much more difficultly the pattern transformation appears. It can be explained that the modulus of the gel increases as the initial chemical potential increases, which is illustrated in Fig.4. The last and the most important one is that, the pattern transformation has a greater influence on mechanical properties of composite material than the water fraction of gel.

3.2. Poisson's ratio

Numerous studies show that the porous material with arrays of holes has negative Poisson's ratio when taking pattern switching. Compared with the negative Poisson's ratio of structure with no gel inside, the pattern switching state exhibits a positive value of the Poisson's ratio in gel composite material with square gel inclusions. Although the Poisson's ratio is positive for the gel composite material, the tendency and shape of gel composite material are same with that of the porous material which was studied by Bertoldi et al (2010) .

The numerical results of Poisson's ratio are plotted as a function of nominal strain in Fig.6 for various values of chemical potential. A strong dependency on this parameter is evident. We find out that the Poisson's ratio of the composite material decreases at which pattern transformation induced by the instability occurs. It is also striking that simply by the decreasing the solvent chemical potential of the gel, composite material can be more easily reconstructed and the Poisson's ratio has a more sharp decline after switching.

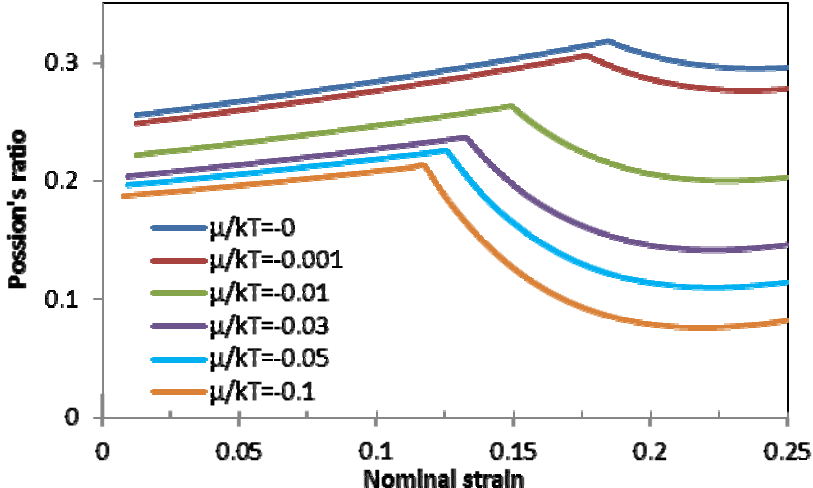


Fig.6 Poisson's ratio as a function of nominal strain using the RVE model with array of square gel inclusions in an elastomeric matrix for various initial chemical potentials.

4. CONCLUSION

We develop the novel composite material by filling the gel inclusions into the periodic elastomeric cellular structures, in which we combine the different shapes of gel material with the PMMA matrix. Numerical simulations of the designed composite material are carried out to investigate the mechanical properties. The behavior of the composite material is characterized by initial almost linear elastic behavior with a sudden change to a different elastic relationship. It can be found that the internal structure of composite material greatly affects mechanical characteristics, so do the different shapes of gel inclusions in composite material. We hope this study can provide future perspectives for this novel composite material, as well as how their properties can be optimized and predicted.

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