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A numerical framework for two-dimensional large deformation of inhomogeneous swelling of gels using the improved complex variable element-free Galerkin method

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ABSTRACT

A numerical framework based on the improved complex variable element-free Galerkin (ICVEFG) method is developed for large deformation analysis of inhomogeneous swelling of gels. In this work, a decomposed free-energy function is derived that avoids the difficulty of treating the chemical potential as a temperature-like variable by changing the chemical potential load into a mechanical load. The Galerkin weak form equation system is derived for inhomogeneous swelling of gels. The essential boundary conditions are imposed through the penalty method. This leads to the corresponding formulae of the improved complex variable moving least-squares (ICVMLS) approximation for 2-D large deformation inhomogeneous swelling of gels. Some example problems of inhomogeneous swelling induced behaviors such as wrinkling, crease and bifurcation are investigated using the developed ICVEFG framework.

1. Introduction

As a kind of soft matter with wide applications, polymeric gels are receiving much attention nowadays. It is a kind of aggregate formed by three-dimensional cross-linked networks of long polymers imbibed in solvent. As the long-chained polymers are capable of large and recoverable deformation, gel swells and shrinks as the solvent molecules migrate in and out as the environment changes. This unique property makes gel a promising material for diverse technologies, such as medical devices [1], drug delivery [2], tissue engineering [3] and actuators [4]. Furthermore, gels are also thought to be a kind of component for life organs [5,6].

Without geometric constraints and mechanical loads, gels swell freely into an isotropic stress-free state but are always under geometric constraints, leading to an inhomogeneous swelling. This inhomogeneous swelling of gels can induce different forms of instability. To model the process of swelling of gels and swelling induced instability, different theories have been proposed [7–17]. Suo et al. [14,15] formulated a theory of coupled mass transport and large deformation in terms of non-equilibrium thermodynamics. This theory determines the state of gels by two fields: (1) the deformation gradient and (2) the solvent concentration. An explicit form of the free-energy function sketches the field in gel equilibrated with

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solvent. Although FEM analyses have been conducted for numerous computational simulation [8–11,15,18,19], the meshless method so far has seldom been used for studying of gels [12,20]. The meshless method is considered to have great advantage in large deformation problems, which is the basic and important attribute of gels [21–29].

As a new generation of numerical tool, the meshless method is wildly used in analyzing nonlinear materials and structures. The element-free kp-Ritz method was proposed by Liew et al. [30] for the large deflection flexural analysis of laminated composite plates. Liew et al. [31] constructed a nonlinear mesh-free formulation for numerical simulation of thermomechanical behaviors of shape memory alloys. Zhao and Liew [32,33] applied the element-free kp-Ritz method for geometrically nonlinear analysis of functionally graded plates and cylindrical shell panels. Lei et al. [34] presented a large deflection analysis of functionally graded carbon nanotube-reinforced composite plates using the element-free kp-Ritz method.

In this paper, a numerical framework based on the improved complex variable element-free Galerkin (ICVEFG) method is proposed for studying inhomogeneous swelling of gels. The ICVEFG method is a novel element-free Galerkin (EFG) method based on the improved complex variable moving least-squares (ICVMLS) approximation [22,23]. The ICVMLS approximation has the advantages inherited from the complex variable moving least-squares (CVMLS) approximation [35]. With the ICVMLS approximation, the trial function of a two-dimensional problem is formed with a one-dimensional basis function. The number of unknown coefficients in the trial function of ICVMLS approximation is less than that in the trial function of MLS approximation. Thus under a same node distribution, the element-free method based on the ICVMLS approximation has higher precision.

For constrained swelling of gel in solvent without mechanical loads, a free-energy function only relying on mechanical deformation gradient is proposed. A multiplication decomposition of deformation gradient is introduced and the free swelled state at chemical potential μ as reference configuration is chosen. The new free-energy function transforms the chemical potential load into mechanical load at a certain chemical potential μ. This paper employs the proposed computational ICVEFG framework for simulating inhomogeneous swelling of gels. The 2-D large deformation weak form control equations are derived by using the proposed new free-energy function. The essential boundary conditions are imposed by the penalty method. All field variables are related to the stress-free free swelling configuration at chemical potential μ. The ICVEFG method is used to test several numerical examples involving inhomogeneous swelling induced wrinkling, crease and bifurcation.

2. An equilibrium field theory of gel

An equilibrium field theory for gel is used as the fundamental material model in this study [15]. A network of polymers is immersed in and imbibes a large quantity of solvent and swells into gel. As illustrated in Fig. 1, gel is immersed in solvent of chemical potential μ that subjects to mechanical loading and geometric constraints. Taking a dry network as the reference state, the point with coordinate $\mathbf{X}$ in the reference state deformed to a location with coordinate $\mathbf{x}(\mathbf{X}, t)$ in the current state at time t. The deformation gradient of the network is

$$\mathbf{F}_{iK} = \frac{\partial x_i(\mathbf{X}, t)}{\partial \mathbf{X}_K}, \tag{1}$$

which describes the deformation of the network. We suppose the solvent concentration in the current state is $C(\mathbf{X})$, which describes the distribution of the solvent molecules in the gel. The deformation gradient $\mathbf{F}$ and the solvent concentration C determine the state of the gel.

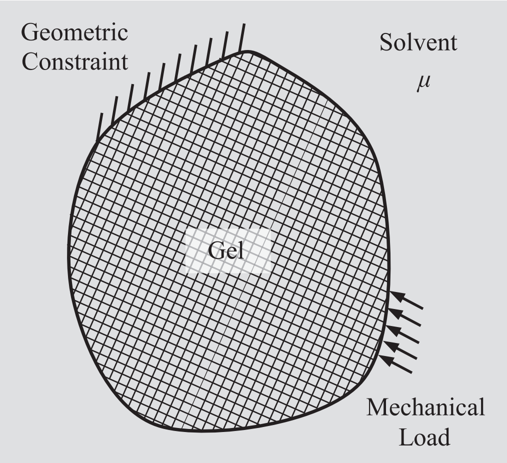

Fig. 1. Gel immerses in solvent of chemical potential μ subjecting to mechanical load and geometric constraints.