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Numerical simulation of mechanical properties in nanoporous membrane

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ABSTRACT

The objective of this work is to understand the surface/interface effect and the size/configuration dependence on the mechanical properties in nanoporous membrane. The stress concentration, nanopores coalescence, effective elastic moduli, damage level, and contraction or expansion areas are numerically investigated in membrane where three representative arrays of nanoporous are taken into account, i.e., parallel, internal, and scatter arrays of multiple nanopores. It is concluded that the surface/interface effect and the size/configuration dependence have a significant influence on the mechanical behaviors. The coalescence path of nanopores may appear along the uni-axial tensile loading direction if the size of nanopores is less than 2 nm due to the surface/interface effect on the nanopores. Variable arrays of nanopores distributed in membrane can result in the different magnitude of effective elastic moduli. The damage level analysis represented by the *M*-integral in views of the energy concept reveals that the parallel arrays of nanopores yields the smallest energy release rate due to the self-similar expansion of nanopores. In particular, the nanopores may be contracted even that the remote tensile loading is applied. These studies present some reasonable explanation of the mechanical behaviors in nanoporous membrane where the mutual or simultaneous influence induced by both the surface/interface effect and the size/configuration dependence.

1. Introduction

Nanoporous materials having pore dimensions on the nanoscale are widely used in engineering structures due to their unique surface, structural, and bulk properties. Nanoporous membranes as a subset of nanoporous materials are receiving considerable attention owing to their particular functional applications. For example, with the development of the ion-track etching technology, nanoporous membranes used as biosensors to deal with the complex biological fluids such as blood or plasma is widely available. The biosensor membranes play an important role in excluding large biomolecules from the blood which could interfere with the measurements, as well as to minimize biofouling [1]. The interesting applications come from the ability of nanopores of certain sizes to let some substances pass and others not, or to force large molecules to pass through one at a time. Various types of nanoporous membranes have been investigated for biosensor applications, including polymeric membranes [2], micromachine silicon membranes [3] and anodic alumina membranes [4]. However, many of these applications focus on the biological properties of nanoporous membranes while in fact most of nanoporous membranes work under the severe mechanical loads. As a result, there would be unexpected deformations and stresses concentration which may affect the durability of the membrane by a sequence of nanopores nucleation, propagation, and coalescence events that accumulate prior to the final failure. Besides, damages induced by stress concentration along multiple nanopores substantially limit the structural integrity and decrease the strength, which will certainly reduce the life time of nanoporous components. Therefore, a variety of challenging issues to the mechanical properties in nanoporous membrane have to be addressed in details.

The main obstacle to investigate the mechanical behaviors in nanoporous membrane is attributed to the surface/interface effect due to high surface-to-volume ratio for nanopores. A generally accepted viewpoint is that the surface/interface effect significantly impacts the phenomenological physical quantities of nanoporous materials such as stress distributions and macro effective elastic moduli significantly. The surface effect that is related to the excess free energy of a surface could be explained by accounting for the surface stress tensors. The conditions imposed at the material surface yield the surface tension, which substantially lead that the surface bond contraction and are critical in analysis of mechanical

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behaviors in nanoporous membrane. Many researchers have already explored the surface/interface effect for multiple interacting nano-inhomogeneities in plane elasticity [5–13]. According to the existing theories, there are two most popular approaches to construct the surface/interface models. One is the thermodynamic framework of solid surfaces proposed by Gibbs [5], such as the atomistic interpretation of interface stress [6], in which an explicit relationship between surface/interface stress and strain is formulated. The other is the continuum surface/interface elasticity described by the Gurtin and Murdoch model [7,8] which is a general theoretical framework for a continuum with surface stresses. In recent years, much attention is focused on the elastic continuum theory to investigate material properties at nanoscale as done by Mogilevskaya et al. [9] who studied the multiple interacting circular nano-inhomogeneities with surface/interface effects by using the Gurtin–Murdoch model.

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The objective of this work is to numerically investigate the surface/interface effect and the size/configuration dependence on the mechanical behaviors in nanoporous membrane. The approach proposed in this paper is referred to the Gurtin and Murdoch model. The emphasis is on the understanding of mechanical behaviors including the stress concentration around the nanopores, the potential coalescence of the neighboring nanopores, the key feature of the macroscopic effective elastic moduli, the damage level characterized by the *M*-integral representing the energy release due to the self-similar expansion of multiple nanopores, the contraction or expansion areas of the nanopores. Three variable arrays of multiple nanopores distributed in membrane are considered in analysis where an infinite elastic plane embedded with parallel, internal, or scatter arrays of nanoporous under a uni-axial tensile loading. The influence of size and configuration on the mechanical properties in membrane is explored. The paper is organized as follows. The complex fundamental solutions for multiple circular holes with surface/interface effects in membrane are explicitly given in Section 2. Numerical results of mechanical properties in nanoporous membrane are presented, and the surface/interface effect and the size/configuration dependence are discussed in details in Section 3. Finally, Section 4 summarizes the concluding remarks.

2. Complex fundamental solutions for multiple nanopores with surface/interface effects in membrane

The stresses and displacements in an infinite, isotropic elastic plane can be evaluated by using the two complex potentials $\varphi(z)$ and $\psi(z)$ as follows [14]:

$$\begin{aligned} &2\mu[u_x(z)+\mathrm{i}u_y(z)]=\kappa\varphi(z)-z\overline{\varphi'(z)}-\overline{\psi(z)},\\ &\sigma_{xx}+\sigma_{yy}=4\mathrm{Re}\varphi'(z),\\ &\sigma_{yy}-\sigma_{xx}+2\mathrm{i}\sigma_{xy}=2[\bar{z}\varphi''(z)+\psi'(z)], \end{aligned} \tag{1}$$

where u_x and u_y are displacements; σ_{xx}, σ_{yy}, and σ_{xy} are stresses; μ and κ are the elastic constants of bulk; $i=\sqrt{-1}$, $z=x+iy$; Re denotes the real part; the over bar and the $\{\prime\}$ denote the complex conjugate and the derivative against z, respectively.

The surface/interface effect that is related to the excess free energy of a surface could be explained by accounting for the surface stress tensors along the nanopores. The conditions imposed at the material surface yield the surface tension and surface elasticity, which are substantially used to solve the problems involving multiple nanoporous. Accordingly, the presence of surface/interface stress should be accounted for in the present work. Applying the model of Gurtin and Murdoch [7] who gave equations that describe the conditions at the surface, the surface energy effect yields the following boundary equations:

$$\mathbf{u}^{inh}=\mathbf{u}^{mat}=\mathbf{u}, \tag{2}$$

$$(\sigma^{inh}-\sigma^{mat})\mathbf{n}=\mathrm{div}_{\sum}\mathbf{S}, \tag{3}$$

$$\mathbf{S}=\sigma_0\mathrm{I}_l+(\lambda_0+\sigma_0)(\mathrm{tr}\varepsilon^{sur})\mathbf{I}_l+2(\mu_0-\sigma_0)\boldsymbol{\varepsilon}^{sur}+\sigma_0\nabla_{\sum}\mathbf{u}, \tag{4}$$

where the superscripts '*inh*' and '*mat*' denote the inhomogeneity nanopores and the matrix, respectively; $\mathbf{n}$ represents a unit normal vector to the surface that points away from the inclusion; $\mathbf{S}$ is the (first) Piola–Kirchhoff surface stress tensor; $\mathrm{div}_{\sum}$ is the surface divergence in its original configuration (before the deformation