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Finite-volume homogenization and localization of nanoporous materials with cylindrical voids. Part 2: New results

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ABSTRACT

The finite-volume homogenization theory with surface-elasticity effects based on the Gurtin-Murdoch model developed in Part 1 is employed to investigate little explored aspects of nanoporous materials' response. New results illustrate the effects of pore array architecture, aspect ratio and mean radius of elliptical porosities on local stress fields and homogenized moduli in an admissible range of porosity volume fractions. These results highlight the importance of adjacent pore interactions neglected in the classical micromechanics models, quantified herein for the first time. The theory is also shown to capture the highly oscillatory stress fields associated with surface-elasticity induced solution instabilities in this class of materials with negative surface moduli without ill-conditioning problems. Differences and similarities between comparable finite-element and finite-volume solutions of the unit cell boundary-value problem are delineated, including identification of pore radii, and associated aspect ratios and volume fractions, at which instabilities initiate. Consistent with reported and herein generated finite-element based results, the solution instability is also shown to depend on finite-volume mesh refinement. Hence care is required to identify the admissible range of parameters in the calculation of homogenized moduli. The new theory provides an alternative and independent means of identifying stable solution ranges, and hence is a good tool in assessing the finite-element method's predictive capability of generating stable solutions. Comparison with molecular dynamics simulations is included in further support of the theory's potential to capture both the initial homogenized response and local stress fields that may lead to failure.

1. Introduction

In Part 2 of this paper we employ the finite-volume direct averaging micromechanics (FVDAM) theory with the surface-elasticity effects implemented in Part 1 based on the Gurtin-Murdoch model (1975) to generate new results on homogenized moduli and local stress fields in nanoporous materials with cylindrical porosities of elliptical cross section (including circular) that highlight the effects of porosity volume fraction, pore radii and shape, and array type. This is a major goal of Part 2 that cannot be properly realized without establishing parameter ranges within which stable solutions are obtained as discussed below. While homogenized moduli of nanoporous materials with circular porosities have been extensively studied using classical micromechanics, finite-element and elasticity-based approaches, just a few papers may be found in the literature that address the effects of elliptical pore aspect ratio and mean pore radius on the homogenized moduli and local stress fields, Javili et al. (2013, 2015), Chatzigeorgiou et al. (2017). As discussed by Winter et al. (2017) in a recent article, pore shape plays a critical role in tuning the properties of nanoporous materials in a wide range of applications. Moreover, even in the case of circular nanoporosities there is little data that addresses the combined effects of porosity volume fraction and nanopore radius on local stress concentrations that affect failure in this class of materials. The classical micromechanics models are not accurate in estimating local stress fields in the medium-high porosity range because they neglect adjacent pore interactions that become important at high porosity content. This is illustrated herein through comparison of the predictions of the widely-used composite cylinder assemblage (CCA) model under biaxial plane strain and axial shear loadings, for which exact solutions are available for both homogenized moduli and local stress fields, with FVDAM results.

We construct unit cells with circular and elliptical cylindrical voids

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Table 1
Elastic moduli of energetic surfaces and bulk matrix of aluminum.

Elastic modulus	Bulk Al matrix	Surface A	Surface B
λ	58.17 (GPa)	3.494 (N/m)	6.851 (N/m)
μ	26.13 (GPa)	− 5.425 (N/m)	− 0.376 (N/m)

in hexagonal and square arrays, and conduct parametric studies aimed at illustrating the combined effects of void shape and mean radius on the full set of homogenized moduli of the two arrays and the related local fields, including high porosity content arrays where pore interaction is important. The elastic moduli for both surface and bulk aluminum matrix taken from Tian and Rajapakse (2007a) that were used in the validation described in Part 1 are also employed in these studies. They are listed in Table 1 for reference. The moduli associated with surface A lead to solution instabilities for mean pore radii of elliptical porosities that are larger than those of circular porosities. Solution instabilities have been reported in dilute and non-dilute nanoporous arrays for both elasticity and finite-element approaches, leading to the ill-conditioning of the governing system of equations for the boundary-value problem, that prevent reliable generation of local stress fields and homogenized moduli below a certain critical pore radius. In the case of elliptical porosities, the mean pore radii below which solution instabilities have been reported also depend on the porosity aspect ratio, Tian and Rajapakes (2007a,b). In contrast, no solution instabilities have been observed for surface B elastic moduli in a wide range of mean pore radii by others as well as the present authors. Therefore in order to generate a reliable set of homogenized moduli, the critical mean pore radius for the given porosity aspect ratio needs to be established.

Hence we also investigate the new theory's solution convergence for surfaces with negative moduli relative to those reported in the literature as a function of the mean pore radius of elliptical porosities, and examine local stress fields associated with surface-elasticity induced apparent bifurcation phenomenon. Little is known about the bifurcation phenomenon in this class of emerging materials despite the wide use of negative surface moduli (obtained from molecular dynamic simulations) in the micromechanics model validation studies discussed in Part 1 of this manuscript. Javili et al. (2012) investigated one type of bifurcation phenomenon that manifests itself as surface wrinkling in homogeneous materials bounded by straight energetic surfaces with negative elastic moduli, and determined closed-form analytical conditions for wrinkling occurrence in terms of the surface and bulk matrix elastic moduli. Using the finite-element approach, these authors also demonstrated that surface wrinkling may occur with mesh refinement or mesh reconfiguration that changes the local element aspect ratios even if the conditions for the bifurcation phenomenon are not met. In contrast, no such analysis appears to be available for nanoporous materials. Hence the conditions for the observed solution instabilities are presently not known and need to be established numerically. This aspect of the analysis of nanoporous materials with energetic surfaces characterized by negative moduli remains to be explored. Part 2 of this paper contributes to this unexplored area by demonstrating the feasibility of using an alternative and independent approach to establish numerically the range of pore radii wherein stable solutions are obtained.

Moreover, the only presently available tool for investigating the bifurcation phenomenon in nanoporous materials is the finite-element method wherein the surface effect is accounted for through additional surface energy which, together with bulk matrix energy, contributes to the total energy of a pore boundary element. These two separate contributions produce an elemental stiffness matrix which is the sum of the bulk matrix and surface parts. For sufficiently small elements and negative surface moduli, the surface contribution may exceed that of the bulk, producing elemental stiffness matrix with negative diagonal elements, Javili et al. (2012), potentially leading to apparent bifurcation. In contrast, the FVDAM theory accounts for the surface effect directly as it employs the elasticity approach in a surface-average sense in the solution of the unit cell boundary-value problem whereby the Young-Laplace equations are explicitly taken into account, see Part 1. Hence the examination of FVDAM solution's stability provides an independent set of data against which the finite-element results may be compared in the quest of identifying causes of the observed solution instabilities. Since comparable finite-element data is not available, we also develop our own finite-element based solution of the unit cell problem for periodic nanomaterials for direct comparison and contrast with the FVDAM results.

This part is organized as follows. In Section 2 we assess solution convergence issues associated with negative surface moduli that produce locally negative surface strain energy to demonstrate the new theory's performance relative to both finite-element and elasticity-based solutions reported in the literature, as well as to the results generated using the in-house finite-element code. The intimately related issue is the emergence of surface instabilities or solution bifurcations in the form of surface stress oscillations that have received little attention in the literature for nanoporous materials. This section provides the basis for establishing the pore radius, aspect ratio and volume fraction ranges for which reliable homogenized moduli and local stress fields may be calculated. The role of the porosity volume fraction on the circumferential stress distribution around the pore boundary in the presence of significant surface-elasticity effects which occur at small pore radii is examined in Section 3. In Section 4 we investigate the effects of elliptical pore aspect ratio and mean radius on the full set of homogenized moduli for two surfaces that lead to decreasing (surface A) and increasing (surface B) homogenized moduli with decreasing mean pore radius. Section 5 presents comparison of molecular dynamics (MD) simulations with FVDAM predictions to highlight both the FVDAM predictive capabilities and areas for further studies. Discussion and conclusions are presented in Sections 6 and 7, respectively. The appendix provides an overview of the finite-element solution of the unit cell boundary-value problem.

2. Solution and surface instabilities

The concepts of material (and related structural) stability have a long history in the study of linearly elastic isotropic materials and related boundary-value problems. They are based either on seeking real solutions to the boundary-value problem involving wave propagation, or incremental solutions from an equilibrium state that do not grow with time. The results of such analyses produce conditions on the elastic moduli that ensure solution stability. Kochmann (2012) provides a concise summary of these conditions. Strong ellipticity, a necessary condition that guarantees stable wave propagation in an isotropic elastic material requires that $\mu > 0$, $\lambda + 2\mu > 0$ in two and three dimensions. A sufficient condition for stability, often referred to as pointwise stability, requires that $\mu > 0$, $\lambda + 2/3\mu > 0$ and $\mu > 0$, $\lambda + \mu > 0$ in two and three dimensions, respectively, noting that the Gurtin-Murdoch surface model is a two-dimensional construct. We also note that for materials with $\mu > 0$, pointwise stability implies strong ellipticity, but the converse is not necessarily true. These conditions may be summarized by requiring that the stiffness tensor must be positive definite, ensuring positive definite strain energy density and hence solution uniqueness to a well-posed boundary-value problem. The loss of pointwise stability may manifest itself in solution bifurcations, including surface wrinkling in homogeneous materials with energetic interfaces.

Instabilities associated with the solution of stress fields in nanoporous materials with surface elasticity effects have been observed for both circular and elliptical porosities when using both finite-element and elasticity-based approaches. Solution instabilities have been reported for circular porosities in square arrays as well as elliptical porosities in an infinite matrix below certain critical pore radii for surface