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Finite-volume homogenization and localization of nanoporous materials with cylindrical voids. Part 1: theory and validation

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Abstract

Surface elasticity effects based on the Gurtin-Murdoch model are incorporated for the first time into a finite-volume based homogenization theory to enable analysis of materials with nanoscale cylindrical voids of circular and ellipsoidal cross-section in periodic arrays. In a departure from the previously employed enforcement of traction and displacement continuity conditions in a surface-average sense applied locally to each subvolume of the unit cell, the Young-Laplace equilibrium equations are implemented using a central-difference approach involving adjacent subvolumes, an approach both new to the finite-volume theory as well as necessary. In Part 1, the new computational capability is validated by published results on homogenized moduli, stress concentrations and full-field stress distributions in nanoporous aluminum obtained using elasticity-based and numerical approaches. Notably, numerical problems associated with singular-like stresses and associated instabilities experienced in finite-element solutions (as well as the elasticity solution of an elliptical void in an infinite matrix) are not as pronounced in the proposed approach, enabling determination of surface and full-field stresses in a wider range of pore radii. New results are generated in Part 2 aimed at demonstrating the effects of nanopore array type and aspect ratio of elliptical voids on homogenized moduli and local stress fields in a wide range of porosity volume fractions and radii. These results highlight the importance of adjacent pore interactions neglected in the classical micromechanics models, that remains to be quantified by numerical homogenization techniques.

Keywords: nanocomposites; surface effects; finite-volume homogenization; homogenized moduli; local stress fields.