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Homogenization and localization of nanoporous composites - a critical review and new developments

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Abstract

Nanoporous materials find a wide range of applications spanning diverse disciplines. For sufficiently small nanopores, surface effects must be accounted for in calculating homogenized moduli and local stress fields. Surface effects are typically simulated using the Gurtin-Murdoch model based on the concept of an infinitesimally thin surface with its own elastic moduli and equilibrium conditions. This paper critically reviews the different approaches employed in the calculation of both homogenized moduli and local stress fields of unidirectional nanoporous materials in a wide range of porosity volume fractions, pore sizes and different array types. These approaches include classical micromechanics, elasticity-based, finite-element and finite-volume techniques. The vehicles for comparison which provide the gold standard are two recently extended homogenization theories with incorporated Gurtin-Murdoch type surfaces. The locally-exact homogenization theory is an efficient elasticity-based approach which accurately yields the full set of homogenized moduli and concomitant local stress fields in rectangular, square and hexagonal porosity arrays of unidirectional nanocomposites. The theory's excellent stability, quick convergence and rapid execution times enable extensive parametric studies to be conducted efficiently. The second homogenization theory is the recently generalized finite-volume direct averaging micromechanics approach. This theory provides greater flexibility in simulating the response of nanoporous materials with arbitrarily shaped porosities, and exhibits herein demonstrated greater range of numerical stability relative to the commonly used finite-element method. New results are generated aimed at demonstrating the effects of nanopore volume fraction, radii and arrays on homogenized moduli, local stress fields and initial yield surfaces. These results highlight the importance of adjacent pore interactions neglected in the classical micromechanics models, which are critically assessed.

Keywords: nanoporous composites; surface effects; elasticity, finite-volume and finite-element based homogenization; homogenized moduli; local stress fields; initial yield surfaces; stability.

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