Computational Grains for Nanocomposites with Interface Stress Effects

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Abstract: In this study, two/three-dimensional computational grains are developed for micromechanical modeling of heterogeneous materials with nanoscale inhomogeneities, considering the interface stress effect. Two types of computational grains are developed, depending on the types of inhomogeneity in each element. Each computational grain can include alternatively a spherical void or a spherical elastic inclusion. In these computational grains, an inter-element compatible displacement field is assumed along the element outer-boundary, and interior displacement fields in the matrix as well as in the inclusion are independently assumed as T-Trefftz trial functions. For planar problems, complex potentials are used to derive the Trefftz trial displacement fields, and for 3D problems spherical harmonics are used as the Papkovich-Neuber potentials to derive the Trefftz trial displacement fields. Characteristic lengths are used to scale the Trefftz trial functions, to avoid ill-conditioning of the derived system of linear equations. The compatibility between the independently assumed displacement fields and the stress jump across the matrix/inclusion interface, described by the generalized Young–Laplace equation, are enforced by Lagrange multipliers in multi-field boundary variational principles. Numerical results by the computational grains with interface stress effects are consistent with available analytical solutions in the literature, demonstrating the high accuracy of the present method. Computational grains for nanocomposites with interface stress effects with ellipsoidal, and arbitrary shaped voids/inclusions will be presented in future studies.

Keywords: Nanocomposites; computational grains; interface stress effect