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AN EXTENDED FINITE ELEMENT METHOD FOR MODELLING MICRO AND NANO INCLUSIONS WITH IMPERFECT INTERFACES

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ABSTRACT

We propose a numerical framework to model the effects of imperfect interfaces between the constituents of heterogeneous media at micro or nanoscale. The aim of this work is to replace thin interphase, whose thickness can be of several orders smaller than the dimensions of heterogeneity, by an equivalent imperfect interface. From a numerical point of view, we avoid the use of volume elements for the interphase, which can be awkward if its thickness is small. An extended finite element formulation in tandem with a level-set method [3,5] is introduced to avoid meshing the interface with surface elements, which is a difficult task for complex three-dimensional geometries.

Two different types of imperfect interfaces are considered. On one hand, in the coherent model, the main variables (temperature or displacements) are continuous across the interface while flux or stress are discontinuous and must satisfy the Laplace-Young equation. On the other hand, in the context of the spring layer model [1], the normal flux or stresses are continuous across the interface, while the temperature or the displacements suffer a jump and are related to the flux or stresses through an appropriate constitutive relationship. The coherent interface model has been widely used to describe surface effects in nanomaterials and nanostractures [2,4] that are due to the large number of surface atoms as compared to their volume counterpart. It can also model a thin interphase between solids with high properties (conductivity or stiffness) compared to the bulk properties, as can be found with coated fibers in composites. The spring layer imperfect interface has been introduced to model thin interphases with low thermomechanical properties. This model can be used to capture the effects of imperfectly bonded particles/fibbers in composites of the effects of transition properties, which occur e.g. in concrete between inclusions and cement paste. Due to the non-constant surface-to-volume ratio as the size of the inclusions change, the surface and bulk energy do not vary in the same proportion. Thus the effective properties of materials containing such imperfect interfaces are usually size-dependent [4]. In contrast to previous works on XFEM where cracks or perfect interfaces were studied, a rigidity term associated with the interface appears. We apply the proposed framework to evaluate the size-dependent effective properties of

heterogeneous materials containing imperfectly bonded interfaces. The use of the extended/level-set framework allows us studying arbitrary shapes of inclusions. Numerical examples are provided with application to determining the size-dependent properties of micro and nanomaterials [6,7]. One direct future application is the study of particular materials composed of randomly distributed inclusions such as e.g. concrete materials.

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