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A nonlocal cohesive zone model for finite thickness interfaces: mathematical formulation, numerical implementation and materials science applications

Although real interfaces between heterogeneous materials have a finite thickness, they are often simplified as boundary layers, i.e., zero-thickness boundaries between the material constituents. Then, cohesive zone models (CZMs) relating the cohesive tractions to the displacement discontinuities are employed for their fracture mechanics characterization. The main drawback of such an approach, widely used in several fields of engineering and materials science, relies in the fact that the shape of the CZM is usually chosen as simple as possible for numerical reasons, rather than being physically based. Therefore, the reliability of these models is a serious concern. To overcome such a drawback, molecular dynamics simulations have been recently applied to determine the stress-separation relations of finite thickness interfaces. However, the extrapolation of these relations to real material microstructures is an open issue.

To overcome such limitations, a nonlocal CZM based on continuum damage mechanics is herein presented to characterize the evolution of damage in the interface region. It is shown that this model provides the proper mathematical framework for interpreting molecular dynamics-based stress-separation relationships that are typically nonlocal, since they always refer to a finite number of atom layers. As a main result, the shape of the nonlocal CZM is found to be a function of damage evolution. Depending on the ductility of the material, different shapes of the CZM can be recovered, from linear and bilinear softening curves, typical of brittle materials, to bell-shaped curves typical of ductile materials. After discussing the numerical implementation of the nonlocal CZM in the finite element method, which requires the use of a nested Newton-Raphson loop for the computation of the tangent stiffness matrix, several engineering applications are proposed. Special focus is given to the simulation of fracture in polycrystalline materials. It is shown that the proposed model is able to produce realistic statistical distributions of Mode I fracture energies, originating from the natural variability of the grain boundary thickness. Moreover, it provides a novel interpretation to the grain size effects on the material tensile strength.

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