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A hierarchical multiscale cohesive zone model and simulation of dynamic fracture in metals

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ABSTRACT

In this work, a hierarchical higher order multi-scale cohesive zone model (MCZM) is developed to simulate the fracture and crack propagation in crystalline solids. The main novelties of the present work are: (1) the hierarchical cohesive zone model is developed, and higher order Cauchy–Born rules (up to the third order) are employed to model different orders of the process zones; (2) the finite element bubble mode is added into the lower order element to capture high-order strain gradient effects in the conventional bilinear quadrilateral element; (3) Barycentric finite element method is used to construct shape functions for hexagonal shaped cohesive zones, and (4) realistic EAM potential is implemented to simulate fracture in metals. Numerical simulations of fracture and crack propagation in both monocrystalline solids and polycrystalline solids are performed. Results show that the crack propagation velocity is in general agreement with that of a corresponding molecular dynamics simulation. Moreover, the transition from intergranular fracture to transgranular fracture in polycrystalline solids is found to be sensitive to both the grain size and the relative grain strength. Finally, it is revealed that the proposed multiscale model can capture the spall fracture in a copper plate under high-speed impact.

1. Introduction

Crystalline materials are extensively used in many engineering branches such as aerospace, civil, mechanical engineering and materials science. The fracture of crystalline materials has been a critical issue in material design, synthesis and performance. The failure mechanics of materials [1,2] has been the focal point of material science. Considering the microstructure of polycrystalline solids, each grain has a unique crystallographic lattice orientation, shape and size, and the grain boundary between two grains is an inhomogeneous interphase with finite thickness. Many researchers, e.g. [3,4], have pointed out that the microstructure of polycrystalline solids has strong influences on how crack propagates in crystalline materials.

To model the fracture in crystalline solids, various methods have been developed at different scales. At macro-scale, there are many classical continuum damage models such as [5–8]. For instance, a temperature dependent creep damage model is proposed to investigate the damage of polycrystalline ice e.g. [9]. As a physical model of continuum damage, micromechanics-based void growth and coalescence models of polycrystalline solids have been extensively studied [10,11]. However, the main drawback of continuum damage models is that these models cannot describe the effects of microstructure characteristics such as lattice orientations and shapes [1,12]. At micro-scale, although ab initio methods or the first principle method are accurate, it is hardly practical to implement them to solve problems of large atomic systems

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Nomenclature

$\mathbf{G}$	gradient of deformation gradient
$\mathbf{H}$	second order gradient of deformation gradient
$\mathbf{F}_e$	element deformation gradient
$\mathbf{P}$	the first Piola–Kirchhoff stress
ϕ	the atomistic potential
$\mathbf{Q}$	the stress couple
$\mathbf{R}_i$	undeformed lattice distance
$\mathbf{S}$	the second Piola–Kirchhoff stress
σ	the Cauchy stress
$\mathbf{U}$	the second order stress couple
$\mathbf{u}(\mathbf{x})$	the displacement field
W	strain energy density

because of the expensive computational cost [13]. Classical molecular dynamics (MD) increases the computational speed substantially but makes a compromise in accuracy compared to the first principle method e.g. [14]. Nevertheless, it is still impossible to conduct simulations of large scale atomistic systems for practical applications. From micro-scale to mesoscale, researchers have proposed many multi-scale methods in order to bridge the atomistic and continuum scales in a consistent manner. For example, a multi-scale boundary element method is proposed to investigate the degradation and fracture in polycrystalline materials [15]. Clayton [1] investigated dynamic thermomechanical response of a tungsten heavy alloy by considering cohesive interaction between adjacent grains.

Since middle 1990s [16], the cohesive zone model (CZM) has been widely used to simulate fractures in solid materials. It is a finite element version of classical cohesive crack model proposed by Dugdale [17] and Barrenblatt [18]. In this model, cohesive zone separates bulk elements automatically based on the magnitude of the external load, and it is governed by the traction-separation cohesive law between two bulk elements. This method has gained much popularity in computational materials failure analysis and mesoscale polycrystalline modeling. However, one prominent drawback of the conventional cohesive zone model lies in the fact that the bulk and cohesive zone constitutive relations are not related, and the empirical cohesive laws may not describe a mixed-mode decohesion mechanism of solids [19]. To overcome this problem, Zeng and Li [20] and Li et al. [21] proposed a multi-scale cohesive zone model, which employs an atomistic potential to construct the constitutive relation of bulk material using the Cauchy–Born rule. In particular, a depletion potential of the cohesive interface is constructed in accord with the atomistic potential inside the bulk material. These potentials naturally take into account the information of lattice microstructure, such as atom positions and lattice orientations. Subsequently, the multi-scale cohesive zone model was utilized to simulate many phenomenons in practice. For example, Qian and Li [2] adopted the multi-scale cohesive zone model to study the crack propagation in polycrystalline solids. Zeng and Li used this method to model composite materials [22]. He and Li [23] combined the embedded atom method (EAM) with cohesive zone model (CZM) to simulate the fracture and crack propagation at mesoscale and macroscale. Liu and Li [24] proposed a finite temperature multi-scale interphase zone model to simulate crack propagation of metallic materials. Fan and Li [25] employed the multi-scale cohesive zone model(MCZM) to study crack propagation in polycrystalline solids, by making use of the higher order Cauchy–Born rules of the same atomistic potential in both the cohesive interface and bulk elements.

There are several differences between the current work and that in [25]. In the original work of Fan and Li [25], a bilinear quadrilateral element was employed to model the cohesive zone element. The deformation inside the process zone is assumed to be inhomogeneous, and the second order Cauchy–Born rule is used to derive the constitutive relation. However, the bilinear quadrilateral element only provides bilinear polynomials, which cannot support the main part of the second order strain gradients, so that the effect by using second-order Cauchy–Born rule based constitutive relation is almost the same as that by using the first-order Cauchy–Born rule based constitutive relation. Therefore, in the present work, a bubble mode is added into the quadrilateral element to support high-order strain gradient effects. Moreover, through mathematical manipulation of integration by parts, an interface cohesive law that is capable of describing the lattice microstructure of the cohesive zone is derived.

In this work, the multi-scale cohesive zone model is constructed in a Lagrange type of the Galerkin finite element weak form formulation. Barycentric finite element method is used to construct shape functions and quadrature integration rules for hexagonal domains. Numerical simulations of fracture in crystalline and polycrystalline solids are carried out. The first example only considers the first-order process zone in polycrystalline solids, while both the first-order and second-order process zone are taken into account in crystalline solids for the second and third example. Finally, the effects of the grain size and the strength ratio between the intergranular fracture to transgranular fracture transition are investigated quantitatively. The critical strength ratio for the transition from intergranular fracture to transgranular fracture is given for different grain sizes.