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Micromechanical boundary element modelling of transgranular and intergranular cohesive cracking in polycrystalline materials

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ABSTRACT

In this paper a cohesive formulation is proposed for modelling intergranular and transgranular damage and microcracking evolution in brittle polycrystalline materials. The model uses a multi-region boundary element approach combined with the dual boundary element formulation. Polycrystalline microstructures are created through a Voronoi tessellation algorithm. Each crystal has an elastic orthotropic behaviour and specific material orientation. Transgranular surfaces are inserted as the simulation evolves and only in those grains that experience stress levels high enough for the nucleation of a new potential crack. Damage evolution along (inter- or trans-granular) interfaces is then modelled using cohesive traction separation laws and, upon failure, frictional contact analysis is introduced to model separation, stick or slip. This is the first time inter- and trans-granular fracture are being modelled together by BEM, and DBEM is being extended to include cohesive approach for anisotropic materials. Finally numerical simulations are presented to demonstrate the validity of the proposed formulation in comparison with experimental observations and literature results.

1. Introduction

Polycrystalline materials are commonly used in many engineering applications. It is then of high technological interest to study how the macroscopic properties of materials such as metals, alloys and ceramics can be enhanced or optimized for specific applications through knowledge of microscopic features. In this work attention is focused on failure mechanisms of brittle polycrystalline materials such as ceramics, where the features and properties of the microstructure play a pivotal role in the elastic response of the whole structure and eventually in its failure. As pointed out by Crocker [1], "even though conceptually a simple process, the description of fracture in materials within ductile or brittle regimes is complex".

Models for describing damage nucleation and growth can be considered over different ranges of length scale: atomistic models are at the lower scale and homogeneous materials at the other extreme [1].

Real fracture processes depend on many synergistic factors. The main features include: grain elastic properties, level of anisotropy and grain orientation, their morphology, grain size distribution within the aggregate, stiffness and toughness mismatch [2]. It is also well recognised that material's crystallography structure affects the initiation of micro-cracking: (1) adjacent grains of non cubic phases can experience differential expansion due to thermal expansion anisotropy (TEA); (2) phase transformation (e.g. tetragonal to monoclinic) can also cause micro-cracking; (3) strain differences due to elastic anisotropy

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Nomenclature

$\mathbf{A}$	sub-matrix of kernel integrals (unknown field)
b	orthotropic parameter
$\mathbf{B}$	sub-matrix of kernel integrals (known field)
$\mathbf{C}$	compliance tensor
d	damage parameter
$\mathbf{D}$	strain kernel tensor
E	Young modulus
$\mathbf{G}$	matrix of traction kernels
$\mathbf{H}$	matrix of displacement kernels
H	generic grain
$\mathbf{I}$	identity matrix
l	side length of square microstructure
$\mathbf{L}$	matrix of strain kernels
$\mathbf{M}$	matrix of stress kernels
r	distance from crack apex
$\mathbf{R}$	rotation matrix
$\mathbf{S}$	stress kernel tensor
t	traction
$\mathbf{T}$	traction kernel tensor
u	displacement
$\mathbf{U}$	displacement kernel tensor
$\mathbf{x}$	field point
α	cohesive parameter
β	cohesive parameter
ε	strain
θ	angular direction from crack apex
λ	loading factor
μ	friction coefficient
ν	Poisson's ratio
σ	stress
τ	shear stress
ϕ	interface angle
Φ	cohesive potential
$a_{1,2}$	orthotropic parameter
$A_{1,2}$	orthotropic parameter
$\bar{A}_{gr}$	average grain area
C_{ij}	Cauchy principal value free term
$\delta\mathbf{u}$	displacement jump
$\delta\mathbf{u}_{n,t}^{crit}$	critical component of displ. jump
δ_{ij}	Kronecker delta
$\delta\lambda$	loading factor increment
$\theta_{1,2}$	orthotropic parameter
$\mu_{1,2}$	eigenvalues of charact. equation
σ_{crit}	critical tensile stress
τ_{crit}	critical shear stress
Φ_0	energy of separation
ASTM G	grain size index
$\mathbf{C}'$	plane strain/stress tensor
$\mathbf{C}^{\mathbf{coh}}$	sub-matrix of cohesive laws
$\bar{d}_{gr}$	average grain size
$E_{1,2}$	modulus of elasticity
$\hat{f}$	transgranular damage
$G(\phi)$	work of separation
G_n	norm. work of separation
G_t	tang. work of separation
$G_{I,II}$	energy release rates
G_{I_c}	critical energy release rate
K_{IC}	fracture toughness
$\bar{L}^f$	average element length

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