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A modelling of microstructure evolution and crack opening in FCC materials under tension

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Certification

I, Nam N. Huynh, declare that this theis is wholly my own work unless otherwise referenced and acknowledged. The document has not been submitted for qualifications at any other academic institution.

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Abstract

The field of fracture mechanics can generally be divided into two groups: (i) the study of material behaviour prior to crack and (ii) the developing of crack opening criteria. Even though various studies have been done in both subjects there are still gaps that need to be bridged. This thesis aims at combining both groups of the modelling of dynamic fracture in crystalline materials at a reasonable cost of computational time.

A model of crystal plasticity finite element method has been formulated to account for the effects of lattice structure in the crystalline materials. The model has been applied to simulate tensile deformation around a notch tip in both single crystals and polycrystalline aggregates. By comparing with observations from various experiments, the model has been proved to be able to accurately capture the material's behaviours around a notch tip undergoing tensile load. Particularly, this model is among the very few, if not the first, that accurately predicts various experimental observations of two notch tip orientations (010)[101] and (010)[100] that are widely found in the literature.

This study has also developed a crack opening criterion that is dependent upon the evolution of the lattice structure. The core of this new criterion is an atomic interaction model that estimates energies of the interface of an fcc bicrystal. Results of grain boundary energy of <100> and <110> symmetrical tilt boundaries of an aluminum bicrystal obtained from the atomic interaction model agree very well with those from molecular dynamics simulations.

The newly developed criterion has been applied to the modelling of crack opening and crack growth in a region around the notch tip in single crystals. Elements in the finite element mesh satisfying the criterion are removed from the mesh by using the element removal technique in Abaqus/Standard. Missing elements effectively act as voids in the material. Thus crack opening (in terms of void nucleation) and the

subsequent crack growth (in terms of coalescence of new and existing voids) are captured naturally. The newly developed methodology to model crack opening has been applied to predict mode I crack growth around a notch tip in Cube and Brass oriented fcc single crystals. The obtained results show similar behaviours of crack growth with those from molecular dynamics simulations of single crystals having the same lattice orientations.

The methodology to model crack opening that has been proposed in this thesis is original. It enables the explicit modelling of crack growth without presuming a crack path. Also, a predefined crack opening criterion, which could be erroneous, that has been used in many finite element simulations of fracture is avoided. To the best of the author's knowledge, the criterion of crack opening that depends on the structure of the interface of two misoriented lattices is presented in this study for the first time.

The current thesis focuses into modelling tensile deformation and the subsequent fracture in fcc crystals. The methodology that has been proposed however can be readily applied to crystalline materials of various lattice structures with minor modifications.

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Table of Contents

Notations

$\otimes$	Tensor product
α^{tilt}, β^{tilt}	Angles defining orientation of tilt axis in the global coordinate system
$\mathbf{\Omega}$	Spin tensor
$\mathbf{\Omega}^{*}$	Lattice rotation of spin tensor
$\mathbf{\Omega}^{p}$	Plastic parts of spin tensor
α^{th}	A slip system α
α^{hkl}	Angle of rotation about a global $[hkl]$ axis
Γ_0	Work of separation
γ	Shear strain of a slip system
γ_0	Reference value of slip
$\dot{\gamma}^{(\alpha)}$	Shear strain-rate caused by the plastic slip in the α^{th} slip system
$\dot{\gamma}_0^{(\alpha)}$	Reference value of shear strain rate
$\delta\mathbf{D}$	Virtual form of the rate of deformation
Δt	Time increment
$\mathbf{\Delta d}_A^i$, $\mathbf{\Delta d}_B^i$	Displacement vectors from time i-1 to time i at points A and B
φ_1, Φ, φ_2	Three Euler angles
δ_n	Corresponding crack opening
$\delta\mathbf{v}$	Kinematically admissible virtual velocity field
$\delta\mathbf{v}^{\mathbf{n}}$	Virtual nodal velocity field
$\boldsymbol{\sigma}$	Cauchy stress
σ_{max}	Peak separation stress
$\dot{\boldsymbol{\sigma}}$	Time derivative of Cauchy stress
$\overset{\nabla}{\boldsymbol{\sigma}}$	Jaumann rate of Cauchy stress on axes rotating with the material
$\boldsymbol{\sigma}_A$, $\boldsymbol{\sigma}_B$	Cauchy stress tensor at points A and B

τ_0	Initial critical resolved shear stress
τ_1	Breakthrough stress where large plastic flow initiates
$\tau^{(\alpha)}$	Resolved shear stress on slip system α.
$\tau_c^{(\alpha)}$	Critical resolved shear stress of slip system α.
a_1	Constants for $f_{\alpha\beta}$ (no junction)
a_2	Constants for $f_{\alpha\beta}$ (Hirth lock)
a_3	Constants for $f_{\alpha\beta}$ (coplanar junction)
a_4	Constants for $f_{\alpha\beta}$ (glissile junction)
a_5	Constants for $f_{\alpha\beta}$ (sessile junction)
$\mathbf{C}_0$	Tensor of elastic moduli
$\mathbf{d}_A^i$, $\mathbf{d}_B^i$	Coordinates of points A and B at time i
$\mathbf{D}$	Stretching tensor
$\mathbf{D}^*$	Elastic part of stretching tensor
$\mathbf{D}^p$	Plastic part of stretching tensor
$\mathbf{D}_L$	Rate of the elastic stretching in the lattice coordinate system
$\mathbf{D}_{\mathbf{gi}}$	Matrix transforming a vector in the global coordinate system to the coordinate system of crystal i
D^{damage}	Damage variable
$\mathbf{E}$	Green strain tensor
E_{crit}	Interface fracture energy of a bicrystal
$\dot{\mathbf{E}}$	Rate of Green strain tensor
$\mathbf{f}$	Surface traction per unit of the current area
$\mathbf{F}$	Total deformation gradient
$\dot{\mathbf{F}}$	Time derivative of the total deformation gradient
$\mathbf{F}^*$	Elastic deformation gradient
$\mathbf{F}^p$	Crystallographic slip on the slip system (plastic deformation gradient)
$f_{\alpha\beta}$	Strength of a particular slip interaction between two slip systems α and β
$\mathbf{F}^{(\alpha)P}$	Contribution of α^{th} slip system to $\mathbf{F}^p$
g	Relaxation factor, which varies from 0 to 1
g^{iso}, h^{iso}, r^{iso}	Isoparametric element coordinates

$\mathbf{H}$ Fourth-order hardening parameter tensor

h_0 Hardening modulus just after initial yield

h_s Hardening modulus during easy glide

$h_{\alpha\alpha}$ Self hardening moduli

$h_{\alpha\beta}$ Instantaneous hardening moduli including self hardening of each system

$\mathbf{I}$ A second-order unit tensor

$\mathbf{K}$ Jacobian matrix

$\mathbf{L}$ Velocity gradient

$\mathbf{L}^*$ Component of velocity gradient due to elastic stretching and lattice rotation

$\mathbf{L}^p$ Plastic contribution of velocity gradient $\mathbf{L}$

$\mathbf{m}^{(\alpha)}$ Normal vector of slip plane of slip system α^{th} in the current configuration

$\mathbf{m}_0^{(\alpha)}$ Normal vector of slip plane of slip system α^{th} in the reference configuration

$\dot{\mathbf{m}}^{(\alpha)}$ Time derivative of the normal vector of a slip system α^{th} in the current configuration

$\mathbf{n}^{\mathbf{intf}}$ Normal vector of the interface of a bicrystal in the global coordinate system

N Number of slip systems

$\mathbf{N}_\mathbf{i}^\mathbf{0}$ Initial normal vectors {111} in the global coordinate system

$\mathbf{N}_\mathbf{i}^\mathbf{k}$ Normal vectors {111} in the global coordinate system at state k

$\mathbf{N}^{(1)}$, $\mathbf{N}^{(2)}$, $\mathbf{N}^{(3)}$ Normal vectors of slip traces from Rice's solutions for fcc crystal

$\hat{\boldsymbol{\rho}}_\mathbf{l}$ Tilt axis with respect to the coordinate system of the fixed lattice

$\hat{\boldsymbol{\rho}}_\mathbf{g}$ Tilt axis in the global coordinate system

$\mathbf{P}^{(\alpha)}$ Symmetric part of Schmid factor

q Latent hardening parameter

$\mathbf{R}$ Orthogonal rotation tensor

$\dot{\mathbf{R}}$ Time derivative of the orthogonal rotation tensor

$\mathbf{R}_\mathbf{i}^\mathbf{k}$ Orientation matrix of crystal i at state k

$\mathbf{R}_{\mathbf{j}}^{\mathbf{k}}$	Orientation matrix of crystal j at state k
$\mathbf{R}_{\mathbf{ij}}^{\mathbf{k}}$	Misorientation matrix between point i and point j
$\mathbf{R}_{L}$	Rotation tensor between the lattice coordinate system and the current configuration
$\mathbf{S}^{(1)}, \mathbf{S}^{(2)}, \mathbf{S}^{(3)}$	Directions of slip traces from Rice's solutions for fcc crystal
$\mathbf{s}^{(\alpha)}$	Slip direction vector of a slip system α^{th} in the current configuration.
$\mathbf{s}_{0}^{(\alpha)}$	Slip direction vector of a slip system α^{th} in the reference configuration.
$\dot{\mathbf{s}}^{(\alpha)}$	Time derivative of slip direction vector of slip system α^{th} in the current configuration
$\mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)}$	Schmid factor
$\mathbf{t_0}$	Kirchhoff stress in the current configuration at the time t
t_n	Normal stress ahead of crack tip for mode I crack
$\dot{\mathbf{t}}$	Material rate of Kirchhoff stress
$\dot{\mathbf{t}}_{0}$	Stress rate in the reference configuration
$\dot{\mathbf{t}}_{1}^{*}$	Rate of the Kirchhoff stress in the intermediate configuration
$\dot{\mathbf{t}}_{L}$	Material rate of the Kirchhoff stress in the lattice coordinate system
$\overset{\nabla}{\mathbf{t}}$	Jaumann rate of Kirchhoff stress on axes that rotate with the material
$\overset{\nabla}{\mathbf{t}}^{*}$	Jaumann rate of Kirchhoff stress on axes that rotate with the lattice
$\mathbf{U}$	Right stretch tensor
$\mathbf{v}$	Velocity in the current configuration
V	Volume of the solid body in the current configuration
$\mathbf{v}^{\mathbf{n}}$	Nodal velocities
$\mathbf{v}_{i}^{n}$	Nodal velocities at iteration step i
$\mathbf{W}^{(\alpha)}$	Asymmetric part of Schmid factor
W_{intf}	Net strain energy on the interface under the effects of external loading
$\mathbf{X}$	Position of material points in the current configuration

List of Figures

List of Tables