Berichte aus dem
Institut für Eisenhüttenkunde

Jinshan He

Microstructure informed modeling of cleavage fracture

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To my family

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Abstract

Cleavage fracture is always an issue since it occurs with “no warning” on many structural steels with different phases and inclusions. These microstructure features have challenged the understanding of micromechanism and predictive capabilities of the conventional cleavage fracture models. The present thesis contributes to the understanding of fracture micromechanism and accurate fracture prediction of a ferritic-pearlitic steel by proposing a new generalized Orowan model. A ferritic-pearlitic steel containing both pearlite and some inclusions is investigated. For this steel, various mechanical tests (e.g. three point bending tests and tensile tests of notched round bar and plane strain samples) were used to achieve different stress states and elastic-plastic finite element method simulations were used to analyze the local stress and strain distributions. Combined with scanning electron microscope and electron backscatter diffraction analysis, the cleavage fracture behavior of the investigated steel is described. In addition, an easy and systematic material parameter calibration procedure with different experiments is proposed for the generalized Orowan model. Good prediction applying the model to the three point bending tests with Charpy specimens for the steel is achieved. This validates the generalized transferability and flexibility of the suggested model for steels under various stress states. The model is also compared with other models, in particular the Beremin model, to address its advantages. As the model is formulated in a phenomenological sense, it however suffers from a drawback: a weak link to the material microstructure. Therefore, a micromechanical model is also proposed linking the microstructure to the phenomenological material parameters. By applying the micromechanical model, microcrack initiation strains of various stress states are extracted and compared with the calibrated results of the macromechanical model. The virtual experiment method is further applied to investigate the microstructure influence on cleavage fracture.

Kurzzusammenfassung

Seit geraumer Zeit stellt der Spaltbruch, welcher in vielen Mehrphasenstählen „ohne Vorwarnung“ auftritt, ein Problem in der industriellen Anwendung dar. Diese Tatsache fordert einerseits ein besseres Verständnis der zurgrunde liegenden Mikromechanismen, andererseits wird die Zuverlässigkeit bestehender Spaltbruchmodelle in Frage gestellt. Die vorliegende Arbeit befasst sich neben der Untersuchung von Mikromechanismen des Spaltbruchs, mit einer präzisen Bruchprognose von ferritisch-perlitischen Stählen durch ein neu postuliertes, verallgemeinertes Orowan-Modell. Aus diesem Grund wurde ein ferritisch-perlitischer Stahl, bestehend aus Ferrit, Perlit und Mangansulfiden, untersucht. Das mechanische Versuchsprogram umfasste unterschiedliche Probengeometrien (z.B. 3-Punkt-Biegeversuche, gekerbte Rundzugproben und Plane Strain Proben), um ein möglich breites Spektrum an Spannungszuständen abbilden zu können. Zudem wurden elastisch-plastische FEM-Simulationen durchgeführt, welche zur Bestimmung lokaler Spannungs- und Dehnungsverteilungen im Werkstoff verwendet wurde.

Mit der zusätzlichen Hilfe von Rasterelektronenmikroskop- und Electron Backscatter Diffraction-Untersuchungen wurde das Spaltbruchverhalten des perlitisch-ferritischen Stahls beschrieben, während zur Parameterkalibration des verallgemeinerten Orowan-Modells ein einfaches und systematisches Versuchsprogramm aufgestellt wurde. Anhand des kalibrierten Modelles konnte eine gute Vorhersage der mechanischen Materialeigenschaften im 3-Punkt-Biegeversuch mit Charpy-Proben erzielt werden, wodurch die Übertragbarkeit und Flexibilität des vorgeschlagenen Modells bestätigt wurde. Des Weiteren wurde ein Modellvergleich durchgeführt, wobei der Fokus auf dem Beremin-Modell lag, um die Vorteile des neuen Modellansatzes zu erläutern. Da das verallgemeinerte Orowan-Modell in einem phänomenologischen Rahmen definiert wurde, ist der Einfluss der Mikrostruktur des Materials auf das Modell gering. Aus diesem Grund wurde ein mikromechanisches Model entwickelt, welches die Mikrostruktur des Werkstoffes mit den phänomenologischen Materialparametern verbindet. Anschließend konnten die durch das mikromechanische Modell bestimmten Mikrorissinitiierungen bei verschiedenen Spannungszuständen mit den kalibrierten Resultaten des makroskopischen Modells verglichen werden. Der letzte Teil dieser Arbeit befasst sich mit virtuellen Experimentmeten, welche zur Untersuchung des Mikrostruktureinflusses auf das Spaltbruchverhalten durchgeführt wurden.

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Notations

Abbreviations

2D	Two-Dimensional
3D	Three-Dimensional
BCC	Body Centered Cubic
BW	Bai Wierzbicki
C3D8R	Continuum 3D 8-node solid element with Reduced integration point
CDM	Continuum Damage Mechanics
CP	Crystal Plasticity
COD	Crack Opening Displacement
EBSD	Electron Back Scatter Diffraction
EDX	Energy Dispersive X-ray spectroscopy
FCC	Face Centered Cubic
FE	Finite Element
FEM	Finite Element Method
ICME	Integrated Computational Materials Engineering
NRB	Notched Round Bar
NRB-R2	Notched Round Bar with 2 mm Radius
NRB-R6	Notched Round Bar with 6 mm Radius
PEEQ	EQuivalent Plastic strain
PS	Plane Strain
RVE	Representative Volume Elements
SEM	Scanning Electron Microscopy
SENB	Single-Edge Notched Bending
SRB	Smooth Round Bar

Symbols

a	Parameter of crystal plasticity model
A_{u}	Uniform elongation
a_{gamma}	Parameter of gamma distribution function
b_{gamma}	Scale parameter of gamma distribution function
C_1–C_4	Parameter of cleavage fracture locus
$\mathbf{C}$	Elastic tensor
D	Damage variable
$D_{\max}$	A parameter of Kolmogorov-Smirnov test
D_{ductile}	Ductile damage variable

d	Half crack length
d'	Grain size
E	Degraded Young's modulus due to damage
E_0	Original Young's modulus
E_p	Plastic deformation energy
E_V	Energy stored in matrix
$E\mathrm{s}$	Surface energy of the crack in the particle
E_t	Tangent modulus of the material
F	Deformation gradient
F^e	Elastic deformation gradient
F^p	Plastic deformation gradient
$\dot{F}_\mathrm{p}$	Rate of plastic deformation gradient
$f_{\mathrm{log-normal}}$	Probability density for log-normal distribution
$f_{\mathrm{gamma}}(x)$	Probability density for gamma distribution
h_0	Initial hardening slope
$h_{\alpha\beta}$	Hardening matrix
$\boldsymbol{I}$	Identity tensor
I_cd	Cleavage damage initiation indicator
I_dd	Ductile damage indicator
$I_1,\ I_2,\ I_3$	The first, second and third stress invariants
j	Sequence number
$J_1, J_2,\ J_3$	The first, second and third invariants for deviatoric stress tensor
L_p	plasticity velocity gradient
l	Diameter of brittle particles
M	Shape factor of the Weibull stress distribution
$M_{\mathrm{log-normal}}$	Location parameter of the log-normal distribution function
m	Shape factor of the Weibull strain distribution
m^α	Slip direction
m^s	Rate sensitivity parameter in the crystal plasticity model
N	Total number of tested samples
n^α	Slip plane normal
P_f	Cumulative probability of failure
$P_\mathrm{f}^{(j)}$	Probability of failure for specimen j
P_nucl	Probability of nucleating a microcrack
P_prop	Probability of propagating the nucleated microcrack
$q_{\alpha\beta}$	Cross-hardening matrix
R_m	Tensile strength
R_eH	High yield point
R_eL	Lower yield point
$S_{\mathrm{log-normal}}$	Scale parameter
t	Thickness of particles
V_i	Volume of the element i
V_0	Reference volume

V_{P}	Fracture process zone
δ_{ij}	Kronecker delta
$\dot{\boldsymbol{\varepsilon}}$	Total strain rate
$\dot{\boldsymbol{\varepsilon}}^{\mathrm{e}}$	Elastic strain rate
$\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}$	Plastic strain rate
$\dot{\bar{\varepsilon}}^{\mathrm{p}}$	Equivalent plastic strain rate
$\bar{\varepsilon}^{\mathrm{p}}$	Equivalent plastic strain
$\bar{\varepsilon}^{\mathrm{p}}_{\mathrm{mci}}$	Microcrack initiation strain
$\varepsilon_{\mathrm{min}}$	Threshold strain value to initiate microcracks
$\bar{\varepsilon}^{\mathrm{p}}_{i}$	Equivalent plastic strain of the element
$\bar{\varepsilon}^{\mathrm{p}}_{\mathrm{ddi}}$	Ductile damage initiation strain
$\bar{\varepsilon}^{\mathrm{p}}_{\mathrm{RVE}}$	The averaged value of equivalent plastic strain over the whole RVE
ε_{u}	Scale parameter of equivalent plastic strain
η	Stress triaxiality
η_{avg}	Average stress triaxiality over loading history
θ	Lode angle
$\bar{\theta}$	Normalized Lode angle parameter
$\bar{\theta}_{\mathrm{avg}}$	Average Lode angle parameter
μ_{gamma}	Mean value for the gamma distribution function
$\mu_{\mathrm{log-normal}}$	Mean value for the log-normal function
ξ	Distance of the origin and the deviatoric plane
ρ	The projection of the vector
$\bar{\sigma}$	Von Mises equivalent stress
σ_0	Initial yield strength
σ_{c}	Critical stress for cleavage fracture
σ_{gamma}	Standard deviation for the gamma distribution function
$\boldsymbol{\sigma}$	Cauchy stress tensor
$\boldsymbol{\sigma}'$	Deviatoric stress tensor
σ_i	Principal Cauchy stress
$\bar{\sigma}^{\mathrm{p}}_{i}$	Equivalent stress of the element i
$\sigma_1^{\mathrm{pearlite}}$	Average maximum principal stress over a pearlite grain
σ_{e}	Effective stress
$\sigma_{\mathrm{e,plane\ stress}}$	Effective stress under plane stress condition
σ_{IC}	Critical maximum principal stress of the particle
$\sigma_{\mathrm{log-normal}}$	Standard deviation of log-normal distribution
$\sigma^{\mathrm{particle}}_{\mathrm{max}}$	Maximum principal stress produced in cementite film
$\sigma^{\mathrm{matrix}}_{\mathrm{flow}}$	Shear flow stress of matrix
$\bar{\sigma}^{\mathrm{p}}_{\mathrm{RVE}}$	Average value of equivalent stress over the whole RVE
σ_{u}	Scaling factors of the Weibull distribution
σ_{w}	Weibull stress
$\sigma_{\mathrm{w,min}}$	Threshold stress value
σ_{y}	Yield stress
γ	Surface energy of unit crack

$\dot{\gamma}$	Plastic multiplier
$\dot{\gamma}_0$	Reference shear rate
γ_p	Plastic energy spent for unit length-crack extension area
$\dot{\gamma}^{\alpha}$	Strain rate of slip system α
$\dot{\gamma}^{\beta}$	Strain rate of slip system β
Φ	Yield function
ν	Poisson's ratio
τ^{α}	Resolved shear stress in α slip system
$\tau^{\alpha}_{\mathrm{crit}}$	Critical resolved shear stress of α slip system
$\tau^{\beta}_{\mathrm{crit}}$	Critical resolved shear stress of β slip system
$\tau^{\mathrm{s}}_{\mathrm{c}}$	Resolved shear stress
τ_0	Initial critical resolved shear stress
τ'_0	Fitting parameter for the grain-size dependent initial critical resolved shear stress
t	Thickness of particles
χ	Aspect ratio of the particle
Λ	Eigenvalue of the stress tensor