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Acta Materialia 59 (2011) 4641–4652

Acta MATERIALIA

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A simulation model for cleavage crack propagation in bcc polycrystalline solids

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Received 24 March 2011; received in revised form 5 April 2011; accepted 6 April 2011
Available online 30 April 2011

Abstract

A model for cleavage crack propagation in a body-centered cubic polycrystalline solid is proposed. The model is based on a criterion that one of the three {1 0 0} cleavage planes in a grain located in front of a crack tip is selected so that normal stress acting on the plane is maximum and the grain is cleaved if the maximum normal stress exceeds the cleavage fracture stress. The normal stress is calculated from mixed mode local stress intensity factors, which are calculated by first-order approximations, where crack surface irregularity, crack front non-straightness and crack closing force acting at ridges between cleavage facets are considered. The calculated fracture surface morphology was compared closely with that of a Charpy impact-tested specimen of low-alloy steel. Ridges formed between the cleavage facets play an important role in the fracture propagation process and fracture surface morphology. The influence of stress triaxiality in the process zone on the extent of fracture surface irregularity is also discussed.

Keywords: Fracture mechanisms; Fracture stress; Micromechanical modeling; Toughness; Ferritic steels

1. Introduction

The prevention of cleavage crack propagation is crucially important in ensuring the integrity of welded steel structures such as ship hulls and cryogenic tanks [1–3]. While many experimental data on crack arrest toughness have been collected by many organizations, little progress has been made to establish a quantitative and universal relationship between steel microstructures and crack arrest toughness based on a physical model of crack propagation.

Many attempts have been made to model crack propagation in solids. In the context of continuum mechanics, stress and strain analyses during dynamic crack propagation have been made both for linear elastic and elastic–plastic solids. The textbooks by Freund [4] and Broberg [5] clearly explain the advances in this field. The behaviors of crack deflection, kinking and branching caused by mechanical conditions and random toughness were analyzed by the finite-element method and integral equations in the context of continuum mechanics [6–10]. Crack propagation behaviors in solids having microstructural characters have also been simulated [11–15]. Kim and Wakayama [11] analyzed grain boundary microcracking and discussed the influences of grain size and grain boundary strength. Kamiya et al. [12] simulated intergranular cracking with a three-dimensional model. Smith et al. [13] modeled ductile-to-brittle transition behavior with a transgranular and intergranular fracture competition model. They also briefly discussed the effect of texture. The influence of dual-phase distribution on the crack path and fracture toughness was modeled for ferrite–carbide steel [14] and Al–SiC [15].

While controlled rolling brings about high crack arrest toughness of steel plates through grain refinement, toughness anisotropy appears especially in heavily controlled rolled steel plates, and this could lower the integrity against cleavage fracture. Crystallographic texture is one of the crucial factors in discussing toughness anisotropy and

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1359-6454/$36.00 © 2011 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
doi:10.1016/j.actamat.2011.04.010

irregularity of crack propagation. Katsuta et al. [16] simulated crack deflection and kinking on the macroscopic scale in a thermomechanically controlled steel plate, assuming toughness directionality. Inagaki et al. [17] calculated the toughness anisotropy of ferritic steels using a cleavage fracture model, in which the relative fracture strength was estimated by taking the grain orientation distribution into account, and compared it with experiments. Yoshinari and Aihara [18] simulated the cleavage crack propagation path with a two-dimensional micromechanical fracture model, on which the present model is based. They assumed that cleavage fracture takes place in a ferrite grain along one of the {1 0 0} planes with maximum normal tensile stress on the planes.

The above-mentioned fracture models are insufficient for describing actual cleavage crack propagation in real body-centered cubic (bcc) polycrystalline solids as represented by ferritic steels; the fundamental aspect of cleavage fracture of {1 0 0} cleavage planes in a crystal grain should be taken fully into consideration. In the present paper, where the discussion is focused on bcc polycrystals, a three-dimensional model which simulates cleavage crack propagation in polycrystalline solids is proposed. Some example calculations are presented and influencing factors on fracture surface morphologies are discussed.

2. Modeling

2.1. Criterion for cleavage fracture of bcc polycrystalline solids

Cleavage fracture takes place on specific crystallographic planes in most metals. The {1 0 0} planes are the most probable cleavage planes in bcc crystals. This presumption can also be applied to polycrystalline bcc solids unless grain boundary strength is so low as to initiate intergranular fracture or twinning takes place, e.g. at extremely low temperatures, below the brittle-to-ductile transition temperature (see Fig. 1). The cleavage fracture criterion in this case may be expressed as

$$\sigma_n \geqslant \sigma_c \tag{1}$$

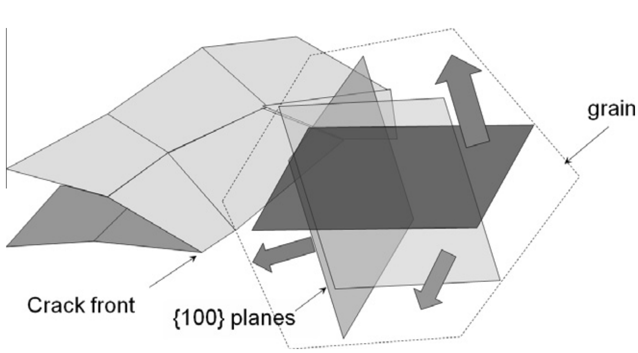

Fig. 1. Possible cleavage plane in a grain in front of a crack tip.

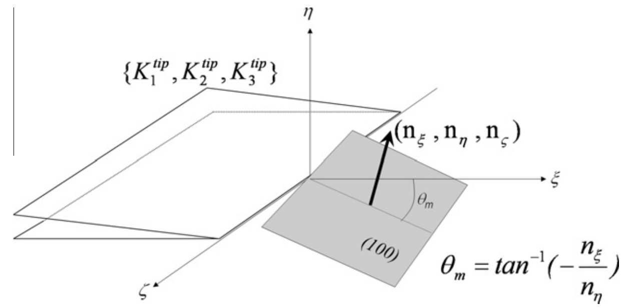

Fig. 2. Definition of the cleavage plane in front of the crack tip.

where σ_n is normal stress acting on the {1 0 0} plane and σ_c is the cleavage fracture stress. The stress tensor in the vicinity of a linear-elastic crack tip is expressed by

$$\sigma_{ij}(r,\theta) = \frac{1}{\sqrt{2\pi r}} K_\alpha^{tip} f_{ij}^\alpha(\theta) \quad (\alpha = 1, 2, 3) \tag{2}$$

where (r, θ) is the polar coordinate, K_α^{tip} is the αth mode of the local stress intensity factor and $f_{ij}^\alpha(\theta)$ are functions of θ [19]. Note that the summation convention applies with respect to α. Suppose that a grain in front of a propagating crack tip is exposed to multiaxial stress, as expressed by Eq. (2) (see Fig. 2). Normal stress acting on the mth {1 0 0} plane ($m = 1, 2, 3$), with unit normal vector $\boldsymbol{n}^{\mathrm{m}}$, is expressed as

$$\sigma_{\mathrm{normal}}^m(r,\theta_m) = n_i^m \sigma_{ij}(r,\theta_m) n_j^m \quad (i, j = \xi, \eta, \varsigma) \tag{3}$$

where θ_m is the incline angle between the crack plane and the {1 0 0} plane concerned, as defined in Fig. 2, and the summation convention applies to i and j (i, $j = 1, 2, 3$). (ξ, η, ζ) are the local coordinates at the crack tip. It is assumed that one of the three {1 0 0} planes is selected so that the normal stress as evaluated by Eq. (3) is maximal. Then the cleavage crack propagates into the grain if

$$\sigma_{\mathrm{normal}}^{\mathrm{max}}(r_c, \theta_m) \geqslant \sigma_c \tag{4}$$

where r_c is the characteristic length. Conceptually, σ_c is the lattice cleavage facture strength and r_c is an order of the lattice parameter of the crystal. However, it is not practical to use these parameters. Then Eq. (4) may be modified as

$$K_{\text{eq-normal}} \geqslant K_{\text{c-local}} \tag{5}$$

where

$$K_{\text{eq-normal}} = \sigma_{\mathrm{normal}}^{\mathrm{max}}(r_c, \theta_m)\sqrt{2\pi\ r_c} = n_i^m [K_\alpha^{tip} f_{ij}^\alpha(\theta_m) n_j^m] \tag{6}$$

$$K_{\text{c-local}} = \sigma_c \sqrt{2\pi r_c} \tag{7}$$

Eq. (5) is used for the crack propagation criterion in the present model by assuming the value of $K_{\text{c-local}}$. Now the problem is reduced to calculating the local stress intensity factors.

2.2. Approximate calculation of local stress intensity factors

In the present model, grains are assumed to be square or rectangular with respect to the global coordinates and are