Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
International Journal of Solids and Structures 42 (2005) 1909–1921
INTERNATIONAL JOURNAL OF SOLIDS and STRUCTURES
www.elsevier.com/locate/ijsolstr

A continuously distributed dislocation model of Zener–Stroh–Koehler cracks in anisotropic materials

X.J. Wu *

Structures, Materials and Propulsion Laboratory, Institute for Aerospace Research, National Research Council of Canada, 1200 Montreal Road, M-13, Ottawa, Ont., Canada K1A 0R6

Received 1 June 2004; received in revised form 15 September 2004
Available online 2 November 2004

Abstract

Based on the continuously distributed dislocation theory (CDDT), the problem of stress equilibrium of a Zener–Stroh–Koehler (ZSK)-type crack in an anisotropic body under mix-mode loading conditions is solved. The solution is obtained for the condition that plastic yielding occurs rectilinearly in front of the crack-tip. The plastic zones size, the crack opening displacements and the energy release rates under mix-mode loading conditions are derived, in closed forms. The orientation dependence in the above quantities is discussed.

1. Introduction

In the early studies on the mechanisms of metal fracture, a concept of crack nucleation was collectively developed by Zener (1948), Koehler (1952) and Stroh (1957). This concept was based on the observation that dislocation pile-ups in front of an obstacle obstructing the propagation of slip bands was in fact the crack nuclei. In the literature, these types of cracks are referred to as Zener–Stroh–Koehler (ZSK) cracks, as summarized by Weetman (1996). To date, such cracks have been treated as if they were in isotropic bodies, even though they are most likely to form in crystalline materials, which have definite slip systems and are generally anisotropic in nature.

As regard to materials with definite slip systems, it is important to realize that material orientation also has a physical effect on crack nucleation and propagation, not only by how much stress is mechanically resolved on the slip plane. In today's engineering, single crystal materials are used as components (from

* Tel.: +1 613 990 5051; fax: +1 613 990 7444.
E-mail addresses: xijia.wu@nrc.ca, xijia.wu@nrc-cnrc.gc.ca

0020-7683/$ - see front matter
doi:10.1016/j.ijsolstr.2004.09.006

Nomenclature

a	crack length
c_i	dislocation distribution length, suffixed with $i = 1,2,3$ for mode II, mode I and mode III, respectively
$B_i(x)$	the ith component of the dislocation distribution vector $\mathbf{B}$(x), $i = 1,2,3$ for glide, climb and screw dislocations respectively
C_{ijkl}	the fourth rank tensor of elastic modulus of the material
u_i	the ith component of the displacement vector $\mathbf{u}$ in a Cartesian coordinate system
σ_{ij}	the stress tensor
s_i	the ith component of the force vector $\mathbf{s} = \{\sigma_{11}, \sigma_{12}, \sigma_{13}\}$ on a plane normal to the x_1 axis, as decomposed from the stress tensor
t_i	the ith component of the force vector $\mathbf{t} = \{\sigma_{21}, \sigma_{22}, \sigma_{23}\}$ on a plane normal to the x_2 axis, as decomposed from the stress tensor
t_i^{F}	the friction resistance in the direction corresponding to t_i
p_α	the material's elastic eigenvalue, $\alpha = 1,2,3$, the root with positive imaginary part
z_α	complex variable, defined as $z_\alpha = x_1 + p_\alpha x_2$ for $\alpha = 1,2,3$
$\mathbf{P}$	a diagonal matrix of p_α
$\mathbf{A}$	$A_{k\alpha}$, a matrix of the material's eigenvectors
$\mathbf{L}$	$L_{i\alpha}$, a 3×3 matrix derived from $L_{i\alpha} = (C_{i2kl} + p_\alpha C_{i2k2})A_{k\alpha}$
$\boldsymbol{h}(z)$	complex field potential of a unit line dislocation
$\mathbf{F}$	the material's characteristic elastic matrix, derived from $\mathbf{F} = -2\mathrm{i}\mathbf{L}\mathbf{L}^{\mathrm{T}}$, where $\mathrm{i} = \sqrt{-1}$ and the superscript 'T' indicates the transpose transformation of the matrix
G	the energy release rate

electronic devices to gas turbine engines) to carry thermomechanical loads. Therefore, study of the behaviour of ZSK cracks in anisotropic materials is important to understand the mechanism and process of crack nucleation in single crystal materials. It is also a precursor of similar studies for polycrystalline materials.

As indicated by Weetman (1996), the ZSK crack and the better-known Griffith–Inglis (GI) crack (Griffith, 1921; Inglis, 1913) form a complementary pair, where a ZSK crack is composed of a symmetric distribution of dislocations, the other crack being asymmetric, according to the Bilby–Cottrell–Swinden model (Bilby et al., 1963), and vice versa in stress distribution along the crack line. A ZSK crack does not close itself when the stresses are removed from the body, as the piling-up Burgers vectors act as the wedge to open the crack, whereas a Griffith–Inglis crack does, ideally. It can be imagined that ZSK cracks may form even under compression, as long as micro-plasticity by slip occurs unevenly due to the presence of microstructural inhomogeneities. This is equivalent to infer that crack nuclei may form under compression, which would have a significant impact on the material's life under low-cycle fatigue conditions (cycling with fully-reversed mechanical strains).

Much attention has been paid to GI-type cracks in the past, because they are more straightforward to deal with in the context of fracture mechanics. Therefore, GI cracks are mostly perceived as the initial flaws in the damage tolerance design philosophy. As pointed out by Zener (1948), GI cracks are not likely to form as the first step in the fracture of metals with the propensity of plastic deformation (crystallographic slip) to ease the stress build up, unless they start at internal pores. It may then be envisaged that GI cracks are present in metals as the result of coalescence of many finer ZSK cracks and/or interactions of the metal with the chemistry of the environment. Many of these microcracking processes occur at a scale below the state-of-the-art non-destructive inspection limit, but they often consume a significant portion of the useful life of a material. In life prediction, crack nucleation and small crack growth are important issues if metal fracture is to be considered as a holistic life process. Mathematical formulations for each stage of the holistic life of a material need to be developed.

To that end, we use the continuously distributed dislocation theory (CDDT) to develop a mathematical formulation for ZSK cracks in general anisotropic materials, studying crack nucleation in metallic materials. The CDDT has been widely applied to deal with point/line-defects in an otherwise homogeneous material, owing to the original work by Eshelby et al. (1953) and later extensions by many other researchers (Stroh, 1958; Bilby et al., 1963; Dundurs and Mura, 1964; Dundurs, 1969; Barnett and Asaro, 1972; Conninou and Dundurs, 1980; Ting, 1986; Suo, 1990; Suo et al., 1992; Hwu and Yen, 1993; Aaundi and Deng, 1995; Ting, 1996; Weetman, 1996; Fulton and Gao, 1997; Wu et al., 2001). The present work is an extension of the previous lines of work on dislocation- based fracture mechanics.

In crystalline materials, slip proceeds on preferred planes (defined by the plane normal n_k) and in definite directions (defined by the slip direction b_k), resulting in the formation of rectilinear persistent slip bands (PSB). It has long been recognized that cracks may nucleate from these PSBs (Thompson and Wadsworth, 1958). Therefore, in the early stage of crack formation when the cracks are small, it is most likely that cracks also form on preferred crystallographic planes in metals. The proceeding of a definite slip system is controlled by the following equation:

$$t_i^{\mathrm{F}} = \sigma_{kl}\mu_{kl}^i \tag{1}$$

where t_i^{F} is the critical resolved shear stress (CRSS), σ_{kl} is the applied stress tensor, and $\mu_{kl}^i = 1/2(b_k^i n_l^i + b_l^i n_k^i)$ is the generalized Schmid factor, and i represent different slip system.

2. The model

In 1958, Stroh (1958) developed an elaborate mathematical formalism for anisotropic elasticity, known as the Stroh formalism, which reduces the stress equilibrium conditions of a solid to an eigenvalue problem. The eigenroots and the eigenvectors are then used to construct characteristic functions of displacements and stresses, as shown in Appendix A.

For a matter of simplicity, in the present treatment we consider an infinite anisotropic medium containing a crack of size $2a$ lying in the plane of $x_1 - x_3(|x_1| < a, x_2 = 0, |x_3| < \infty)$. We assume that dislocations are continuously distributed over the range $[-c_i, c_i]$, as described by the density function vector (numbers of Burgers vectors per unit length)

$$\mathbf{B}(x) = \{B_1(x), B_2(x), B_3(x)\}^{\mathrm{T}} \tag{2}$$

where the subscripts $i = 1, 2, 3$ designates the edge-glide, edge-climb and screw dislocations, corresponding to modes II, I, and III, respectively, as schematically shown in Fig. 1. In this crack configuration, for the convenience of description, the coordinate x_1 is set in parallel with the crack direction, x_3 parallel with the crack front, and x_2 perpendicular to the crack plane. The applied stresses are also defined in reference to this coordinate system. Henceforth, the friction stresses in the x_1 and x_3 directions could be directly related the CRSS of the corresponding slip system. But, the friction stress in x_2 direction, t_2^{F}, is a normal stress component, it is only understood in a generalized sense as the resistance to plastic yield in the specified direction. For example, if the crack formation is a result of the operation of duplex slip systems, the nominal yield stress can be determined from the favourable Schmid relation. Such evaluations are pertinent to particular crystal types, which is out of the scope of the present paper. The present theory is a generalized mathematical treatment for distributed dislocations leading to the formation of rectilinear cracks.

The distributed dislocations on the crack plane satisfy the conditions: (i) the total force exerted by these distributed dislocations produces a net-zero stress ($t_i = 0$) along the crack surface $[-a, a]$ and, (ii) it

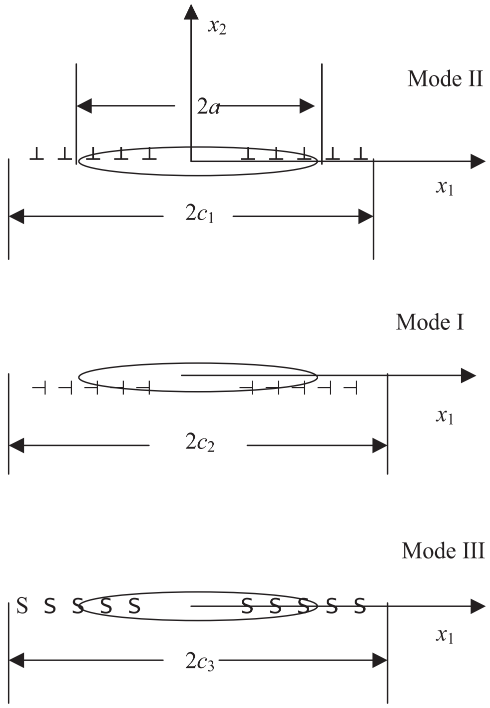

Fig. 1. Schematic representation of modes I, II, III cracks with climb, glide and screw dislocations.

produces a negative yield ($t_i = -t_i^{\mathrm{F}}$) in the region $[-c_i, -a]$ and a positive yield ($t_i = t_i^{\mathrm{F}}$) in the region $[a, c_i]$. These conditions are summarized in the following equation (Weetman, 1996):

$$t_i(x_1) = \begin{cases} t_i^{\mathrm{F}} & a < x_1 < c_i \\ 0 & -a < x_1 < a \\ -t_i^{\mathrm{F}} & -c_i < x_1 < -a \end{cases} \tag{3}$$

For mode I, the "positive/negative yield" means yield in tension/compression respectively, while in modes II and III, the sense is just relative to the reference coordinate. When the crack occurs as the result of operation of a single slip system, it is in a shearing mode (modes II or III), then t_i^{F} is the critical resolved shear stress for that particular slip system. Mode I cracks (in metals), however, are more likely the result of multiple slips or duplex slips, then the corresponding "friction resistance", t_2^{F}, can be determined using the Schmid law, Eq. (1), based on the slip systems involved. In practical cases, for example, the slip-band cracking examined by Thompson and Wadsworth (1958) at the early stage of fatigue was most likely in shearing modes, even the specimen was under uniaxial tension; whereas long cracks in polycrystalline materials and cracks lying on a symmetrical plane of single crystals, such as the (0 1 0) plane in face centred cubic materials, under uniaxial tension are mode-I cracks. For all these cases, in general, t_i^{F} could be deduced from the yield criteria. Therefore, t_i^{F} can be regarded as material constants. Generally, they would need to be determined from physical experiments on internal friction or dislocation velocity measurements or deduced from mechanical testing of single crystal material specimens under simple tension or in shearing. In theory, they can also be estimated based on the Peierls–Nabarro mechanism for single-phase materials (e.g. pure metals) or its modifications when precipitation of second phase occurs in an alloy as the additional strengthening mechanism (Hirth and Lothe, 1982).

On the other hand, the collective force exerted by the continuously distributed dislocations at any point $x_1(x_2 = 0)$ can be expressed by:

$$t_i(x_1) = \int_{-c_i}^{c_i} \frac{F_{ij}B_j(\xi)\mathrm{d}\xi}{2\pi(x_1 - \xi)} \tag{4}$$

where t_i is the vector force acting on the crack plane (Appendix A), F_{ij} is the material's characteristic matrix defined in Appendix A (A.6), and ξ is the coordinate variable over the range $[-c_i, c_i]$.

For equilibrium, we have

$$\int_{-c_i}^{c_i} \frac{F_{ij}B_j(\xi)\mathrm{d}\xi}{2\pi(x_1 - \xi)} = \begin{cases} t_i^{\mathrm{F}} & a < x_1 < c_i \\ 0 & -a < x_1 < a \\ -t_i^{\mathrm{F}} & -c_i < x_1 < -a \end{cases} \tag{5}$$

Generally, when the crack is under a mixed mode condition, there exists an order of dominance, $a < c_i \leqslant c_j \leqslant c_k$ $(i \neq j \neq k)$, and Eq. (5) can be solved by that order. As an example, without losing generality, we shall seek the solution for the condition of $a < c_3 \leqslant c_1 \leqslant c_2$, which applies to the case of mode-I dominance. Then, each dislocation distribution component can be solved using Muskhelishvili's equations (1953) (details are given in Appendix B). The solutions are given as follows:

The plastic zone sizes for modes I, II and III are defined, respectively, as

$$\sqrt{c_2^2 - a^2} = \frac{F_{2j}b_{\mathrm{T}}^{(j)}}{4t_2^{\mathrm{F}}} \quad (j = 1, 2, 3) \tag{6a}$$

$$\sqrt{c_1^2 - a^2} = \frac{b_{\mathrm{T}}^{(1)} + M_{1J}^{-1}F_{J3}b_{\mathrm{T}}^{(3)}}{4M_{1J}^{-1}t_J^{\mathrm{F}}} \quad (J = 1, 2) \tag{6b}$$

$$\sqrt{c_3^2 - a^2} = \frac{b_{\mathrm{T}}^{(3)}}{4F_{3j}^{-1}t_j^{\mathrm{F}}} \quad (j = 1, 2, 3) \tag{6c}$$

and the dislocation distribution functions are given as

$$B_2(x_1) = \frac{2F_{22}^{-1}t_2^{\mathrm{F}}}{\pi}\psi(x_1, c_2) - F_{22}^{-1}F_{21}B_1(x_1) - F_{22}^{-1}F_{23}B_3(x_1) \quad |x_1| < c_2 \tag{7a}$$

$$B_1(x_1) = \frac{2M_{1J}^{-1}t_J^{\mathrm{F}}}{\pi}\psi(x_1, c_1) - M_{1J}^{-1}F_{J3}B_3(x_1) \quad |x_1| < c_1 \tag{7b}$$

$$B_3(x_1) = \frac{2F_{3j}^{-1}t_j^{\mathrm{F}}}{\pi}\psi(x_1, c_3) \quad |x_1| < c_3 \qquad (j = 1, 2, 3; J = 1, 2) \tag{7c}$$

where

$$\psi(x, c) = \ln\left|\frac{\sqrt{c^2 - a^2} + \sqrt{c^2 - x^2}}{\sqrt{c^2 - a^2} - \sqrt{c^2 - x^2}}\right| \tag{8}$$

F_{ij}^{-1} are the elements of the inverse matrix of $\mathbf{F}$, M_{ij}^{-1} are the elements of the inverse of a principal submatrix of $\mathbf{F}$ defined by Eq. (B.12) in Appendix B, and $b_{\mathrm{T}}^{(i)}$ are the total Burgers vector in each respective direction.

Eq. (6) shows that the total length of dislocation distribution, c, in a particular mode is affected by dislocation pile-ups in other modes, due to the anisotropic elastic coupling, so is true for the plastic yielding zone size, which equals to $c - a$. The dislocation distribution functions, as given by Eq. (7), in general, also consist of multiple pile-ups for modes of higher dominance. The elementary distribution function, i.e.,

$\varphi(x_1, c_i)$, represents one dislocation pile-up, symmetrical about the crack centre, with extreme (to the infinity) density at $x_1 = \pm a$, and vanishing at the endpoints of the plastic zone, $x_1 = \pm c_i$. In general, the magnitudes of these quantities in an anisotropic material depend on the orientation of the materials, since they are related to F_{ij} and t_i^{F}, as described in the framework of the Stroh formalism and Hill's theory of plasticity.

The displacement discontinuity, as an accumulation of the Burgers vector, can be calculated by the following integral:

$$u_i = -\int_{-c_i}^{x_1} B_i(x)\mathrm{d}x \quad |x_1| < c_i \tag{9}$$

From Eq. (9) it is derived

$$u_3 = \frac{2F_{3j}^{-1}t_j^{\mathrm{F}}}{\pi}\{a\varphi(x_1, c_3) - x_1\psi(x_1, c_3) + \chi(x_1, c_3)\} \quad |x_1| < c_3 \tag{10}$$

$$u_1 = \frac{2M_{1J}^{-1}t_J^{\mathrm{F}}}{\pi}\{a\varphi(x_1, c_1) - x_1\psi(x_1, c_1) + \chi(x_1, c_1)\} - M_{1J}^{-1}F_{J3}u_3(x_1) \quad |x_1| < c_1 \tag{11}$$

$$u_2 = \frac{2F_{22}^{-1}t_2^{\mathrm{F}}}{\pi}\{a\varphi(x_1, c_2) - x_1\psi(x_1, c_2) + \chi(x_1, c_2)\} - F_{22}^{-1}F_{21}u_1(x_1) - F_{22}^{-1}F_{23}u_3(x_1) \quad |x_1| < c_2 \tag{12}$$

$$(j = 1, 2, 3;\ J = 1, 2)$$

$$\varphi(x, c) = \ln\left|\frac{a\sqrt{c^2 - x^2} + x\sqrt{c^2 - a^2}}{a\sqrt{c^2 - x^2} - x\sqrt{c^2 - a^2}}\right| \tag{13}$$

$$\chi(x, c) = 2\sqrt{c^2 - a^2}\left(\frac{\pi}{2} - \sin^{-1}\frac{x}{c}\right) \tag{14}$$

The crack-tip opening displacements can be obtained, by taking the values from Eqs. (10)–(12) at $x_1 = a$, as:

$$u_3(a) = \frac{4F_{3j}^{-1}t_j^{\mathrm{F}}}{\pi}\left[\sqrt{c_3^2 - a^2}\left(\frac{\pi}{2} - \sin^{-1}\frac{a}{c_3}\right) - a\ln\frac{c_3}{a}\right] \tag{15}$$

$$u_1(a) = \frac{4M_{1J}^{-1}t_J^{\mathrm{F}}}{\pi}\left[\sqrt{c_1^2 - a^2}\left(\frac{\pi}{2} - \sin^{-1}\frac{a}{c_1}\right) - a\ln\frac{c_1}{a}\right] - M_{1J}^{-1}F_{J3}u_3(a) \tag{16}$$

$$u_2(a) = \frac{4F_{22}^{-1}t_2^{\mathrm{F}}}{\pi}\left[\sqrt{c_2^2 - a^2}\left(\frac{\pi}{2} - \sin^{-1}\frac{a}{c_2}\right) - a\ln\frac{c_2}{a}\right] - \frac{F_{21}}{F_{22}}u_1(a) - \frac{F_{23}}{F_{22}}u_3(a) \tag{17}$$

3. Discussion

In the above section, we have obtained the general solution for a ZSK crack with plastic strip-yielding in an anisotropic material under the mixed mode I, II and III conditions showing that $a < c_3 \leqslant c_1 \leqslant c_2$. Interests may lie in some special cases, which are discussed separately below.

3.1. Isotropic cases

For isotropic materials, **F** is a diagonal matrix with $F_{11} = F_{22} = \mu/(1 - \nu)$ and $F_{33} = \mu$, where μ is the shear modulus and ν is the Poisson's ratio. It is then easy to verify that our solution, in the form of Eqs. (6) and (7), reduces to that obtained by Weetman (1996)

$$B_i(x_1) = \frac{2\alpha_i t_i^{\mathrm{F}}}{\pi\mu}\psi(x_1, c_i) \tag{18}$$

$$\sqrt{c_i^2 - a^2} = \frac{\mu b_{\mathrm{T}}^{(i)}}{4\alpha_i t_3^{\mathrm{F}}} \tag{19}$$

where $\alpha_{1,2} = (1 - v)$, and $\alpha_3 = 1$.

In this case, there is no coupling between the different modes of fracture.

Comparing our solution with that known for isotropic materials, it is interesting to note that in an anisotropic material, there is a general coupling of I–II–III modes of fracture. Since the "strength" of a pure ZSK crack is controlled by the dislocation pile-up accumulations, the mode dominance is therefore dependent upon the total Burgers vector in the respective direction. In this paper, we have dealt with the situation of mode-I dominance with $a < c_3 \leqslant c_1 \leqslant c_2$ implying that $b_{\mathrm{T}}^{(3)} \leqslant b_{\mathrm{T}}^{(1)} \leqslant b_{\mathrm{T}}^{(2)}$. Other cases can be solved in a similar manner. In general, the dislocation distribution and the crack-opening displacement of the higher mode of dominance are increasingly affected by dislocations of lesser mode(s), as compared to its counterparts in a similar isotropic material, due to the coupling effect of elastic anisotropy.

3.2. Elastic cases

In the limiting case when $t_i^{\mathrm{F}} \to \infty$ then $c_i (i = 1, 2, 3) \to a$, which means that the dislocation distributions are limited within the crack length in an elastic material. The distribution functions, Eqs. (7), then reduces to

$$B_i(x_1) = \frac{b_{\mathrm{T}}^{(i)}}{\pi\sqrt{a^2 - x_1^2}} \tag{20}$$

which is identical to that in isotropic elastic materials (Weetman, 1996).

The elastic stress ahead of the crack-tip can be calculated as

$$t_i^A(x_1) = \int_{-a}^{a} \frac{F_{ij}B_j(\xi)\mathrm{d}\xi}{2\pi(x_1 - \xi)} = \frac{F_{ij}b_{\mathrm{T}}^{(j)}}{2\pi\sqrt{x_1^2 - a^2}}\left[1 - \frac{2}{\pi}\tan^{-1}\frac{\sqrt{x_1^2 - a^2}}{a}\right] \tag{21}$$

with the stress intensity defined as

$$K_i = \lim_{x_1 \to a}\sqrt{2\pi(x_1 - a)}t_i(x_1) = \frac{F_{ij}b_{\mathrm{T}}^{(j)}}{2\sqrt{\pi a}} \tag{22}$$

Unlike a GI crack whose intensity does not vary with material anisotropy, the stress intensity of a ZSK crack does vary with the material's anisotropic properties, i.e., it is orientation-dependent. As such, nucleation and growth of ZSK cracks in crystalline materials are expected to be orientation-dependent.

It is also interesting to examine the elastic energy release rate, as obtained from the Irwin closure integral, as follows:

$$G = \lim_{\Delta a \to 0}\frac{1}{2\Delta a}\int_{a}^{a+\Delta a} t_i^A(x)u_i(a + \Delta a - x)\mathrm{d}x = \frac{b_{\mathrm{T}}^{(i)}F_{ij}b_{\mathrm{T}}^{(j)}}{8\pi a} = \frac{1}{2}K_iF_{ij}^{-1}K_j \tag{23}$$

Since the matrix F_{ij}^{-1} is positive definite (the determinant of the matrix is positive), the energy release rate is non-negative for all loading conditions. It is also noted that the elastic energy release rate of a ZSK crack, when expressed in terms of the stress intensities, is identical to that of a GI crack. However, unlike a GI crack, which tends to become unstable once its energy release rate ($\sim\sigma^2 a$) reaches a critical value, the formation of a ZSK crack is self-stabilized, since its energy release rate is inversely proportional to the crack size, $2a$. This means that crack propagation would lower the energy of a ZSK crack, if the corresponding piled-up Burgers vectors were held constant.

3.3. Small-scale-yielding conditions

Another interesting case is the so-called small-scale-yielding condition, i.e., $(c_i - a)/a \ll 1$. Then, Eqs. (15)–(17) reduce to

$$u_3(a) = \frac{\left[b_{\mathrm{T}}^{(3)}\right]^2}{8\pi a F_{3j}^{-1} t_j^{\mathrm{F}}} \tag{24}$$

$$u_1(a) = \frac{\left[b_{\mathrm{T}}^{(1)} + M_{1J}^{-1} F_{J3} b_{\mathrm{T}}^{(3)}\right]^2}{8\pi a M_{1J}^{-1} t_J^{\mathrm{F}}} - M_{1J}^{-1} F_{J3} u_3(a) \tag{25}$$

$$u_2(a) = \frac{\left[F_{2j} b_{\mathrm{T}}^{(j)}\right]^2}{8\pi a F_{22} t_2^{\mathrm{F}}} - \frac{F_{21}}{F_{22}} u_1(a) - \frac{F_{23}}{F_{22}} u_3(a) \tag{26}$$

and the energy release rate, G, can be obtained from the Irwin closure integral

$$G = t_i^{\mathrm{F}} u_i(a) \tag{27}$$

A numerical example of dislocation distributions resulting into formation of a ZSK crack on a (1 1 1) plane in a single crystal Ni-base superalloy (ignoring the γ' precipitates) is given below.

The elastic compliances of f.c.c. Ni are (Nye, 1957)

$$s_{11} = s_{22} = s_{33} = 0.00799\ (\mathrm{GPa})^{-1}$$

$$s_{12} = s_{23} = s_{31} = -0.00312\ (\mathrm{GPa})^{-1}$$

$$s_{44} = s_{55} = s_{66} = 0.00844\ (\mathrm{GPa})^{-1}$$

Choosing the Cartesian coordinates xyz as: x—$[1\,\bar{1}\,0]$, y—$[1\,1\,1]$ and z—$[1\,1\,\bar{2}]$ (by convention, x is the crack direction, y is the direction perpendicular to the crack, and z the anti-plane axis), the eigen-matrix F^{-1} an be solved, following the procedures outlined in Appendix A or given in detail in the book by Ting (1996), as

$$F^{-1} = \begin{bmatrix} 0.00889 & 0 & -0.00267 \\ 0 & 0.00802 & 0 \\ -0.00267 & 0 & 0.01397 \end{bmatrix} (\mathrm{GPa})^{-1}$$

The material friction resistances are estimated (based on the yield properties of SRR99 studied by Li and Smith, 1995) to be

$$t_1^{\mathrm{F}} = 530\ \mathrm{MPa},\ t_2^{\mathrm{F}} = 839\ \mathrm{MPa},\ t_3^{\mathrm{F}} = 492\ \mathrm{MPa}$$

Suppose that total accumulations of Burgers vectors took place in the order of $b_{\mathrm{T}}^{(1)}/a = 0.02$, $b_{\mathrm{T}}^{(2)}/a = 0.05$, and $b_{\mathrm{T}}^{(3)}/a = 0.02$, the respective dislocation density function could be determined by Eq. (7), and distribution is shown in Fig. 2. For comparison, the mode I distribution in a would-be isotropic material with the stiffness close to that of the Ni-base superalloy in the respective direction is also shown. It can be seen that there is practically no difference between the isotropic material and the anisotropic material

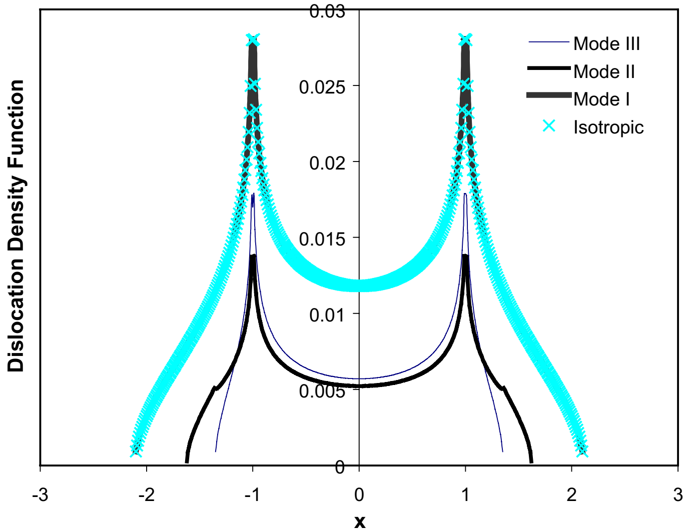

Fig. 2. Dislocation distributions for a mix-mode ZSK crack.

in the dominant mode (in this case, mode I) as long as the moduli are matching for the respective mode. However, there are differences in the modes II and III, even though, the total Burgers vector accumulations are equal for the two modes. This is due to the elastic anisotropic coupling, as shown in the F^{-1} matrix. The coupling, of course, is dependent on the orientation of the crystal with respective to the load. The effect will become important particularly in mixed-mode situations, which are mostly true for crack nucleation conditions. Since the degree of coupling is determined from the eigen-matrix F^{-1} for the particular material/orientation, it is hard to further generalize on this point. Due considerations should be given to this though, when studying crack behaviour in anisotropic materials.

4. Conclusion

Elastic–plastic fracture mechanics formulations have been derived for a Zener–Stroh–Koehler crack of mixed I–II–III modes in anisotropic materials, using the CDDT approach. Closed form expressions of CTOD and the energy release rate, G, are obtained, which are dependent upon the elastic–plastic properties of the anisotropic crystalline material, via its characteristic matrices, F_{ij}^{-1} and t_i^{F}, and their limiting cases of pure elasticity and small-scale yielding conditions are also discussed.

In light of the above discussion, the effect of material anisotropy should be considered when studying crack nucleation in the form of ZSK cracks, as well as GI cracks. At a fine microstructural scale, the effect of crystalline orientation will manifest, no matter if the bulk material is polycrystalline or is a single crystal. Further numerical studies for specific alloy systems shall be pursued in future work.

Acknowledgement

The work was conducted as part of the New Initiative Fund research in the Institute for Aerospace Research, National Research Council of Canada. Constructive discussions with Dr. W. Deng of General Motors Canada Limited are appreciated.

Appendix A. The Stroh Formalism

For the plane strain problems of a homogeneous anisotropic elastic body where displacements and stress depend only on the in-plane coordinates x_1 and x_2, a general representation for the displacement vector **u**, and the stresses **s** and **t**, can be expressed in terms of a complex field potential vector $\mathbf{h}(z)$ by the Stroh formalism, as (Stroh, 1958; Ting, 1996)

$$\begin{aligned}\mathbf{u} &= \{u_1, u_2, u_3\}^{\mathrm{T}} = \mathbf{A}\mathbf{h}(z) + \overline{\mathbf{A}}\overline{\mathbf{h}(z)} \\ \mathbf{s} &= \{\sigma_{11}, \sigma_{12}, \sigma_{13}\}^{\mathrm{T}} = -\mathbf{L}\mathbf{P}\mathbf{h}'(z) - \overline{\mathbf{L}\mathbf{P}}\overline{\mathbf{h}'(z)} \\ \mathbf{t} &= \{\sigma_{21}, \sigma_{22}, \sigma_{23}\}^{\mathrm{T}} = \mathbf{L}\mathbf{h}'(z) + \overline{\mathbf{L}}\overline{\mathbf{h}'(z)}\end{aligned} \tag{A.1}$$

where **A** and **L** ($L_{i\alpha} = [C_{i2k1} + p_\alpha\, C_{i2k2}]\, A_{k\alpha}$) are 3×3 non-singular material matrices, and **P** is a diagonal matrix of three complex eigenvalues p_α ($\alpha = 1, 2, 3$, $\mathrm{Im}(p_\alpha) > 0$). The complex variable z is defined as $z = x_1 + px_2$.

This set of equations satisfies the equilibrium condition:

$$C_{ijkl}u_{k,lj} = 0 \tag{A.2}$$

Hence, the material's eigenvalues p_α ($\alpha = 1, 2, 3$) should satisfy the sextic equation

$$|C_{i1k1} + pC_{i1k2} + pC_{i2k1} + p^2C_{i2k2}| = 0 \tag{A.3}$$

and the eigenvectors satisfy

$$(C_{i1k1} + p_\alpha C_{i1k2} + p_\alpha C_{i2k1} + p_\alpha^2 C_{i2k2})A_{k\alpha} = 0 \quad \alpha = 1, 2, 3 \tag{A.4}$$

For a unit line dislocation **b**, the elementary field potential, in the absence of a line tension force, is given by Koehler, 1952

$$\mathbf{h}(z) = \frac{1}{2\pi i}\langle \ln z \rangle \mathbf{L}^{\mathrm{T}}\mathbf{b} \tag{A.5}$$

where $\langle f(z)\rangle = \mathrm{diag.}[f(z_1), f(z_2), f(z_3)]$ and 'i' is the imaginary unit ($\mathrm{i} = \sqrt{-1}$).

In the Stroh formalism, a matrix, **F**, is defined as

$$\mathbf{F} = -2\mathrm{i}\mathbf{L}\mathbf{L}^{\mathrm{T}} \tag{A.6}$$

which has been proven to be real and positive-definite.

Appendix B. The solutions of Eq. (5) under Conditions $a < c_3 < c_1 < c_2$

Eq. (5) involves multi-length integrals with coupling induced by the anisotropic elasticity, which seems to be difficult to solve directly. Actually, taking advantage of the condition, $B_i(x_1) = 0$ when $|x_1| > c_i$, the integrations over the shorter intervals $[\pm c_1]$ and $[\pm c_3]$ can be extended to $[\pm c_2]$, without altering the integration results. In this case, the equilibrium equations for a ZSK can be written as

$$\int_{-c_2}^{c_2} \frac{F_{1j}B_j(\xi)\mathrm{d}\xi}{2\pi(x_1 - \xi)} = t_1(x_1), \quad |x_1| < c_1 \tag{B.1}$$

$$\int_{-c_2}^{c_2} \frac{F_{2j}B_j(\xi)\mathrm{d}\xi}{2\pi(x_1 - \xi)} = t_2(x_1), \quad |x_1| < c_2 \tag{B.2}$$

$$\int_{-c_2}^{c_2} \frac{F_{33}B_3(\xi)\mathrm{d}\xi}{2\pi(x_1-\xi)} = t_3(x_1), \quad |x_1| < c_3 \tag{B.3}$$

where

$$t_i = \begin{cases} t_i^{\mathrm{F}} & a < x_1 < c_i \\ 0 & -a < x_1 < a \\ -t_i^{\mathrm{F}} & -c_i < x_1 < -a \end{cases} \tag{B.4}$$

Because of the condition $a < c_3 < c_1 < c_2$, the solution should be sought for dislocations with the smallest distribution size first, and then to the next size until the final, i.e., the largest size, is solved.

The governing equation for $B_3(x_1)$ is given as

$$\int_{-c_3}^{c_3} \frac{B_3(\xi)\mathrm{d}\xi}{2\pi(x_1-\xi)} = F_{3j}^{-1}t_j(x_1) = \omega_3(x_1) \tag{B.5}$$

The solution of this integral equation, which is bounded at $x_1 = \pm c_3$, can be obtained, directly using Muskhelishvili's (1953) method, in the following form:

$$B_3(x_1) = -\frac{2\sqrt{c_3^2 - x_1^2}}{\pi} \int_{-c_3}^{c_3} \frac{\omega_3(\xi)\mathrm{d}\xi}{(x_1-\xi)\sqrt{c_3^2-\xi^2}} \tag{B.6}$$

and, $\omega_3(x_1)$ should also satisfy the condition (Weetman, 1996)

$$\int_{-c_3}^{c_3} \frac{x_1\omega_3(x_1)\mathrm{d}x_1}{\sqrt{c_3^2 - x_1^2}} = \frac{b_{\mathrm{T}}^{(3)}}{2} \tag{B.7}$$

where $b_{\mathrm{T}}^{(3)}$ is the total burgers vector along the x_3 coordinate.

Eq. (B.6) leads to

$$B_3(x_1) = \frac{2F_{3j}^{-1}t_j^{\mathrm{F}}}{\pi}\psi(x_1, c_3) \quad (j = 1,2,3) \quad |x_1| < c_3 \tag{B.8}$$

where

$$\psi(x, c) = \ln\left|\frac{\sqrt{c^2-a^2} + \sqrt{c^2-x^2}}{\sqrt{c^2-a^2} - \sqrt{c^2-x^2}}\right| \tag{B.9}$$

while Eq. (B.7) results in

$$\sqrt{c_3^2 - a^2} = \frac{b_{\mathrm{T}}^{(3)}}{4F_{3j}^{-1}t_j^{\mathrm{F}}} \tag{B.10}$$

To solve for $B_1(x_1)$, we rearrange Eqs. (B.1) and (B.2), such that

$$\int_{-c_1}^{c_1} \frac{B_1(\xi)\mathrm{d}\xi}{2\pi(x_1-\xi)} = \omega_1(x_1) = M_{1J}^{-1}\left(t_J(x_1) - \int_{-c_3}^{c_3} \frac{F_{J3}B_3(\xi)\mathrm{d}\xi}{2\pi(x_1-\xi)}\right) \quad (J = 1,2) \quad |x_1| < c_1 \tag{B.11}$$

where matrix $\mathbf{M}^{-1}$ is the inverse of a principal submatrix of $\mathbf{F}$, as defined by

$$\mathbf{M}^{-1} = \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix}^{-1} \tag{B.12}$$

Noting that **F** is real symmetric and positive definite, so is the matrix **M**. Then, substituting Eq. (B.8) into Eq. (B.11), and also using Muskhelishvili's method, we obtain

$$B_1(x_1) = \frac{2M_{1J}^{-1}t_J^{\mathrm{F}}}{\pi}\psi(x_1,c_1) - M_{1J}^{-1}F_{J3}B_3(x_1) \quad |x_1| < c_1 \tag{B.13}$$

while c_1 satisfies the condition

$$\int_{-c_1}^{c_1} \frac{x_1\omega_1(x_1)\mathrm{d}x_1}{\sqrt{c_1^2 - x_1^2}} = \frac{b_{\mathrm{T}}^{(1)}}{2} \tag{B.14}$$

Substituting Eq. (B.11) into Eq. (B.14) and noting that

$$\int_{-c_1}^{c_1} \frac{x\mathrm{d}x}{\sqrt{c_1^2 - x_1^2}} \int_{-c_3}^{c_3} \frac{F_{J3}B_3(\xi)\mathrm{d}\xi}{2\pi(x_1 - \xi)} = -\int_{-c_1}^{c_1} F_{J3}B_3(\xi)\mathrm{d}\xi \int_{-c_3}^{c_3} \frac{x\mathrm{d}x}{2\pi(\xi - x_1)\sqrt{c_1^2 - x_1^2}} = -\frac{F_{J3}b_{\mathrm{T}}^{(3)}}{2} \tag{B.15}$$

we find

$$\sqrt{c_1^2 - a^2} = \frac{b_{\mathrm{T}}^{(1)} + F_{J3}b_{\mathrm{T}}^{(3)}}{4M_{1J}^{-1}t_J^{\mathrm{F}}} \quad (J = 1,2) \tag{B.16}$$

Finally, for $B_2(x_1)$, it follows from Eq. (B.2) that

$$\int_{-c_2}^{c_2} \frac{B_2(\xi)\mathrm{d}\xi}{2\pi(x_1 - \xi)} = \omega_2(x_1) \quad |x_1| < c_2 \tag{B.17}$$

where

$$\omega_2(x_1) = F_{22}^{-1}\left(t_2(x_1) - \int_{-c_1}^{c_1} \frac{F_{21}B_1(\xi)\mathrm{d}\xi}{2\pi(x_1 - \xi)} - \int_{-c_3}^{c_3} \frac{F_{23}B_3(\xi)\mathrm{d}\xi}{2\pi(x_1 - \xi)}\right) \tag{B.18}$$

The solution of Eqs. (15) and (16) can be obtained as

$$B_2(x_1) = \frac{2F_{22}^{-1}t_2^{\mathrm{F}}}{\pi}\psi(x_1,c_2) - F_{22}^{-1}F_{21}B_1(x_1) - F_{22}^{-1}F_{23}B_3(x_1) \quad |x_1| < c_2 \tag{B.19}$$

From the condition

$$\int_{-c_2}^{c_2} \frac{x_1\omega_2(x_1)\mathrm{d}x_1}{\sqrt{c_2^2 - x_1^2}} = \frac{b_{\mathrm{T}}^{(2)}}{2} \tag{B.20}$$

we determine that

$$\sqrt{c_2^2 - a^2} = \frac{F_{2j}b_{\mathrm{T}}^{(j)}}{4t_2^{\mathrm{F}}} \tag{B.21}$$

References

Aaundi, A., Deng, W., 1995. Rigid inclusions on the interface between two bonded anisotropic media. J. Mech. Phys. Solids 43, 1045–1058.

Barnett, D.M., Asaro, R.J., 1972. The fracture mechanics of slit-like cracks in anisotropic elastic media. J. Mech. Phys. 20, 353–366.

Bilby, B.A., Cottrell, A.H., Swinden, K.H., 1963. The spread of plastic yield from a notch. Proc. R. Soc. London A 272, 304–314.

Conninou, M., Dundurs, J., 1980. On the behavior of interface cracks. Res. Mech. 1, 249–264.

Dundurs, J., 1969. Elastic interaction of dislocations with inhomogeneities. In: Mura, T. (Ed.), Mathematical Theory of Dislocations. The American Society of Mechanical Engineers, New York, pp. 70–115.

Dundurs, J., Mura, T., 1964. Interaction between an edge dislocation and a circular inclusion. J. Mech. Phys. Solid 12, 177–189.
Eshelby, J.D., Read, W.T., Shockley, W., 1953. Acta. Metall. 1, 252–259.
Fulton, C.C., Gao, H., 1997. Electric nonlinearity in fracture of piexoelectric ceramics. ASME Appl. Mech. Rev. 50, S56–S63.
Griffith, A.A., 1921. The phenomenon of rupture and flow in solids. Proc. R. Soc. London A 221, 163–197.
Hirth, J.P., Lothe, J., 1982. Theory of Dislocations, second ed. Krieger Publishing Co., New York, pp. 217–242.
Hwu, C., Yen, W.J., 1993. On the anisotropic elastic inclusions in plane elastostatics. ASME J. Appl. Mech. 60, 626–632.
Inglis, G.E., 1913. Stresses in a plate due to the presence of cracks and sharp corners. Trans. Inst. Naval Archit. 55, 219–230.
Koehler, J.S., 1952. The production of large stresses by dislocations. Phy. Rev. 85, 480–481.
Li, S.X., Smith, D.J., 1995. Temperature and Orientation dependence of elastic and yield properties of single crystal nickel base superalloy. Mater. Sci. Tech. 11, 1253–1260.
Muskhelishvili, N.I., 1953. Some Basic Problems of the Mathematical Theory of Elasticity. Noordhoff, Leyden.
Nye, J.F., 1957. Physical Properties of Crystals. Oxford University Press.
Stroh, A.N., 1957. A theory of the fracture of metals. Adv. Phys. 6, 418–465.
Stroh, A.N., 1958. Dislocations and cracks in anisotropic elasticity. Philos. Mag. 3, 625.
Suo, Z., 1990. Singularities, interfaces and cracks in dissimilar anisotropic media. Proc. R. Soc. A 427, 331–358.
Suo, Z., Kuo, C.-M., Barnett, D.M., Willis, J.R., 1992. Fracture mechanics for piezoelectric ceramics. J. Mech. Phys. Solids 40, 739–765.
Thompson, N., Wadsworth, J.J., 1958. Metal fatigue. Adv. Phys. 7, 72–169.
Ting, T.C.T., 1986. Explicit solution and invariance of the singularities at an interface crack in anisotropic composites. Int. J. Solids Struct. 22, 965–983.
Ting, T.C.T., 1996. Anisotropic Elasticity: Theory and Applications. Oxford University Press, Oxford.
Weetman, J., 1996. Dislocation Based Fracture Mechanics. World Scientific, Singapore.
Wu, X.J., Deng, W., Koul, A.K., Immarigeon, J.-P., 2001. A continuously distributed dislocation model for fatigue cracks in anisotropic crystalline materials. Int J. Fatigue 23, S201–S206.
Zener, C., 1948. The micro-mechanism of fracture. In: Fracturing of Metals. American Society for Metals, Cleveland, pp. 3–31.