Influence of Crystal Grain on Stress Intensity Factor of Microstructurally Small Cracks*

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Abstract

If crack size is in the order of several grain diameters or smaller, the stress intensity factor (SIF), which brings about change in crack growth behavior, is affected by various factors caused by the grain. For example, kinks and bifurcations of cracks at grain boundary triple points vary the SIF when the crack runs along grain boundaries. The elastic anisotropy of crystals and inhomogeneous stress distribution at the microstructural level in a polycrystalline body also bring about changes in the SIF. In this paper, such influences of the crystal grain on the SIF are reviewed. Firstly, the SIF of kinked or branched cracks is outlined. Secondly, the SIF of cracks in an anisotropic body as well as inhomogeneous polycrystalline body is summarized. In particular, statistical changes in SIF are shown as a function of crack size. Finally, based on the results obtained, statistical changes in the SIF and their influence on the growth of the microstructurally-small-crack are discussed.

Key words: Stress Intensity Factor, Crystal Grain, Grain Boundary, Microstructure, Polycrystal, Crack Path

1. Introduction

Stress intensity factor (SIF) is a parameter representing the magnitude of the stress field in the vicinity of a crack tip, and usually exhibits a good correlation with the crack growth rate in fatigue and stress corrosion cracking (SCC)⁽¹⁾⁽²⁾. Once the correlation is experimentally obtained, the crack growth behavior in a component can be predicted by evaluating the SIF. Empirical relationships have been investigated for various materials and environments⁽²⁾⁻⁽⁴⁾, and applied to prediction of crack growth in order to ensure the integrity of plant components⁽⁴⁾⁻⁽⁷⁾. The SIF of cracked components can be evaluated by numerical calculations or with use of a handbook⁽⁸⁾⁽⁹⁾, which lists the SIFs for various crack shapes and boundary conditions.

If crack size is in the order of several grain diameters or smaller, SIF needs to be carefully evaluated, since it is usually affected by microstructure. For example, when a crack runs along grain boundaries, it is not straight as illustrated in Fig. 1. The crack exhibits kinks and bifurcations even in the cases of transgranular cracking. This causes change in the magnitude of SIF. The magnitude of the change depends on geometrical factors, including deflection angle, length, and others. When a crack is sufficiently large, by averaging the SIF along the crack front, the microstructural effects on the magnitude is negligible; namely macroscopic cracking behavior. However, it has significant influence on

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Fig. 1 Typical cracks in polycrystalline body.

the crack growth in the microstructurally-small-crack. In the case of three-dimensional cracks, in particular, the change in SIF differs along the crack front depending on the grain structure.

The SIF in a body with anisotropic elasticity is not always the same as that evaluated under the assumption of isotropic elasticity. Due to constraint in deformation around the crack tip, the SIF of a surface crack varies depending on the degree of anisotropy of elasticity. The microstructural inhomogeneity of polycrystalline material also causes changes in the SIF. Although the macroscopic behavior of polycrystalline materials is isotropic and homogenous in terms of elastic deformation when materials have random crystallographic and morphologic texture, the anisotropic property of each crystal produces nonuniform stress at the microstructural level (hereinafter termed local stress) even under conditions of uniform remote stress ⁽¹⁰⁾⁻⁽¹²⁾. Therefore, the SIF of the microstructurally-small-crack is affected by the inhomogeneous stress distribution.

Since the SIF of the microstructurally-small-crack in a polycrystalline body is affected by several factors, it is important to evaluate precisely the SIF in order to understand the growth behavior. In this paper, the authors present a review of the published data of the influence of crystal grains on the SIF of microstructurally-small-cracks. First, the influences of crack shape are summarized, and then the SIF of cracks in an anisotropic body as well as inhomogeneous polycrystalline body is reviewed.

2. Influence of change in crack shape due to crystal grain

2.1 Two-dimensional cracks

2.1.1 SIF of kinked cracks

Figure 2 shows typical patterns with kink(s) or bifurcation of two-dimensional cracks. In cases of simple kinking (Fig. 2(a)), the SIF can be calculated by the following equations ⁽¹³⁾⁽¹⁴⁾.

$$\begin{aligned} k_1(\alpha) &= C_{11}(\alpha)K_I(a) + C_{12}(\alpha)K_{II}(a) \\ k_2(\alpha) &= C_{21}(\alpha)K_I(a) + C_{22}(\alpha)K_{II}(a) \end{aligned} \quad (1)$$

where K_I and K_{II} are the SIFs of Modes I (opening model) and II (shear mode) without kink, respectively, and k_1 and k_2 are those of a kinked crack, α is the angle of deflection of the

Fig. 2 Patterns with kinks or bifurcation in two-dimensional crack.

kink, and a is the length of the crack. The coefficients C_{ij} are given by ⁽¹³⁾

$$\begin{aligned} C_{11}(\alpha) &= \frac{3}{4} \cos\left(\frac{\alpha}{2}\right) + \frac{1}{4} \cos\left(\frac{3\alpha}{2}\right) \\ C_{12}(\alpha) &= -\frac{3}{4} \left\{ \sin\left(\frac{\alpha}{2}\right) + \sin\left(\frac{3\alpha}{2}\right) \right\} \\ C_{21}(\alpha) &= \frac{1}{4} \left\{ \sin\left(\frac{\alpha}{2}\right) + \sin\left(\frac{3\alpha}{2}\right) \right\} \\ C_{22}(\alpha) &= \frac{1}{4} \cos\left(\frac{\alpha}{2}\right) + \frac{3}{4} \cos\left(\frac{3\alpha}{2}\right) \end{aligned} \quad (2)$$

These equations can be derived from the stress field near the crack tip by assuming that the length of the kink, b , is negligibly small compared to the length of the main crack, a . Figure 3 shows the relationship between the SIFs k_1 and k_2 and the deflection angle α . The Mode I SIF decreases as the deflection angle increases. It falls to less than 40 percent of that for a straight crack ($\alpha = 0$). In the case of intergranular cracking of SCC, the angle of deflection can be more than 60° , and decreases in the SIF due to the deflection make the crack growth rate slow or arrested the growth of microstructurally-small-cracks ⁽¹⁵⁾. On the other hand, the Mode II SIF increases even under pure tensile loading, although the maximum Mode II SIF is smaller than the Mode I SIF in the range of $\alpha < 90^\circ$. It is in general difficult to say how much of the crack growth is due to the Mode II SIF because of the closure and friction of crack faces ⁽¹⁶⁾.

Fig. 3 Change in Mode I and II components of SIF due to kink near the crack tip under remote tensile stress ($b \ll a$).

Fig. 4 Change in SIF of Mode I due to kink under remote tensile stress.

Fig. 5 Ratio of SIF of Mode I and II at kinked crack tip under remote tensile stress.

When the crack continues to grow after kinking, the ratio b/a increases. The SIF of a kinked crack with finite b/a was obtained⁽¹³⁾⁽¹⁶⁾⁻⁽²³⁾, and Figs. 4 and 5 show the relationships between k_1/K_1 , k_2/k_1 and b/a ⁽¹⁶⁾. The change in Mode I SIF does not significantly depend on the length of deflection, b/a . On the other hand, Mode II SIF increases as b/a increases, and is more than twice the Mode I SIF when $b/a > 0.5$ and $\alpha > 60^\circ$. It was shown that the SIF for the other side (tip “B” in Fig.2(a)) is almost the same as K_1 even under $b/a = 2.0$ ⁽¹⁷⁾.

In the case of doubly-kinked cracks (Fig. 2(b)), when $b_1 \ll a$ and $b_2 \ll b_1$, the local SIF at the crack tip, $k_i^{(2)}$, can be expressed as follows under remote tensile loading⁽²⁴⁾⁽²⁵⁾:

$$k_i^{(2)} = C_{1j}(\alpha_1)C_{ji}(\alpha_2)K_1 \quad (3)$$

Figure 6 shows the magnitude of $k_1^{(2)}/K_1$ for various combinations of α_1 and α_2 ⁽²⁴⁾. In the case of $\alpha_1 = \alpha_2 = 30^\circ$, the SIF is almost the same as K_1 . Namely, Mode I SIF is the maximal when the angle of deflection of the kinked tip is perpendicular to the loading direction. Similar tendency was observed for cracks with large deflection angle α_1 , although

Fig. 6 Stress intensity factors of the doubly-kinked crack under remote tensile stress
($b_1 \ll a, b_2 \ll b_1$).

Fig. 7 Stress intensity factors of the zigzag shaped crack under remote tensile stress.

Fig. 8 Stress intensity factors of the trapezoidal shaped crack under remote tensile stress.

maximum SIF decreased as the angle of deflection increases.

SIFs were calculated numerically for cracks with zigzag and trapezoidal shape⁽²⁰⁾⁽²²⁾⁽²⁶⁾⁻⁽³⁰⁾. Figure 7 shows the SIF of a zigzag-shaped crack obtained by the body force method (BFM) under remote tensile loading⁽³⁰⁾. Although the SIF depends on the angle of deflection α , the number of kinks has minor influence on the Mode I component. The broken lines in Fig. 7 show the SIF of a kinked crack obtained by Eq.(1) with the assumption of angle of deflection α . The SIF of the zigzag-shaped crack is almost the same as that of the kinked crack with the same angle of deflection.

Figure 8 shows the SIF of a crack with trapezoidal shape⁽³¹⁾. The SIF decreases when the crack tip is on the inclined path, while it is almost equivalent to that of a straight crack when the tip is on the horizontal path. In addition, the SIF at the inclined path is almost the same as that of the kinked crack with the same angle of deflection, which is shown by the broken line. It is concluded that the angle of deflection of the crack tip is predominant to the change in SIF regardless of the number of kinks and the overall shape of the crack.

2.1.2 SIF of branched cracks

For branched cracks, several solutions are available ⁽¹⁸⁾⁽³²⁾⁻⁽³⁷⁾. Figure 9 shows the SIF of a crack with symmetric bifurcation with various branch angles ⁽³⁵⁾. Isida and Noguchi obtained a power series formulation of SIF for branched cracks in terms of b/a and branch angle β based on analysis results by BFM ⁽³⁵⁾. As seen for the kinked crack, Mode I SIF decreases as branch angle increases, and approaches $1/2^{0.5}K_I$ for infinitesimally small branch angle β ⁽³³⁾. Therefore, bifurcation of the crack tip decreases crack growth rate regardless of the branching angle. Mode II SIF is small for branching angle $\beta = 0^\circ \sim 30^\circ$. The change in SIF at crack tip "B" (Fig. 2(e)) due to bifurcation is insignificant, as discussed for kinked cracks ⁽³³⁾.

The SIF of a crack with asymmetric branch lengths has also been evaluated ⁽³²⁾⁽³³⁾⁽³⁵⁾. Figure 10 shows with branch angle $\beta = 45^\circ$ ⁽³⁵⁾. The SIF of the longer branch is larger than other one, and is almost constant when the relative length b_2/b_1 is less than 0.5. On the other hand, the SIF of the shorter branch strongly depends on relative length, and decreases towards zero as length decreases. As the difference in the SIF points out the promotion of further unbalance in the lengths in a crack growth process, the shorter branch will be left behind from the main crack. Since bifurcation reduces the SIF regardless of the angle and length of branching, crack growth may decelerate at a triple point of grain boundaries.

Fig. 9 Stress intensity factors of branched crack tip with symmetric bifurcation under remote tensile stress.

Fig. 10 Stress intensity factors of branched crack tip with asymmetric bifurcation under remote tensile stress.

Fig. 11 Kink and twist of the three-dimensional crack tip.

Fig. 12 Stress intensity factor of surface crack with undulated front under remote tensile stress.

Kitagawa et al. pointed out that a so-called plateau region in the relationship between the SIF and SCC growth rate could be caused by the decreases in SIF due to the bifurcation⁽³³⁾.

Although we focus on the results obtained under pure tension in the current review, the SIF of kinked and branched crack under conditions of bi-axial stress⁽³⁵⁾ and shear stress⁽¹⁷⁾⁽³⁵⁾ were also evaluated.

2.2 Three-dimensional cracks

In a three-dimensional field, not only crack kink but also twist must be taken into account, as shown in Fig. 11(a). The change in SIF due to the kink, twist and their combination can be expressed as follows⁽²⁵⁾,

$$k_i = f_{ij}(\alpha, \phi) K_j \quad (4)$$

where α and ϕ are the angles of the kink and twist, respectively. K_j is the SIF when $\alpha = \phi = 0$. Mode III SIF must be considered in the equation. The coefficients f_{ij} were obtained by assuming the extension length b to be negligibly small⁽²⁵⁾, and results showed that Mode I SIF decreased as the angle of twist and kink increased.

Moreover, as shown in Fig. 11(b), the variation in the SIF along the crack front should be taken into account. When the crack front faces several grains, the SIF may vary

Fig. 13 Stress intensity factors of semi-circular surface crack in a single nickel crystal of different crystal orientation under remote tensile stress. Crystal orientation is defined by the Eulerian angle: $(\theta_1, \theta_2, \theta_3)$ (unit: deg.) illustrated in the figure.

depending on the geometry of grains at each position, resulting in deformation of the front shape. The SIF of a nonplanar surface crack has been investigated ⁽³⁸⁾⁽³⁹⁾, and recent software enables us to derive the SIF of three-dimensional cracks with arbitrary geometries ⁽⁴⁰⁾. The SIF along the front of a three-dimensional crack is sensitive to undulation of the crack front ⁽⁴¹⁾⁻⁽⁴⁶⁾. Figure 12 shows the SIFs of surface cracks with a smooth undulated front generated from a cosine function, together with that of a semi-circular crack ⁽⁴⁷⁾. SIFs become large and small at points of denting and bulging, respectively. The magnitude of deviation from that of a semi-circular crack is dependent on the curvature and height of the dent, meaning that the crack tends to become semi-circular. The average of the SIF along the crack front is almost the same as that of a semi-circular crack of the same radius. Therefore, if a crack is large enough, growth in area is almost equivalent to that of a semi-elliptical crack of the same area regardless of the non-uniform SIF distribution.

3. Influence of anisotropy of crystal grain

3.1 SIF in anisotropic single crystals

Anisotropy of materials has little effects on the SIF in general ⁽⁴⁸⁾⁻⁽⁵⁰⁾, and no effect in an infinite and orthotropic plate ⁽⁵⁰⁾. The SIF for a compact tension specimen made from an anisotropic single crystal is almost identical to that for an isotropic body ⁽⁵¹⁾. However, in the case of kinked cracks ⁽⁵²⁾ or surface cracks ⁽⁵³⁾⁻⁽⁵⁷⁾, the SIF in an orthotropic single crystal is obviously different from that in an isotropic body. Hashimoto et al. examined the SIFs of semi-circular surface cracks in a single crystal that had various crystal orientations by finite element analysis (FEA), and found that SIF strongly depended on crystal orientation ⁽⁵³⁾⁽⁵⁴⁾. Figure 13 shows the SIF of a semi-circular surface crack in a single nickel crystal subjected to remote tensile loading ⁽⁵⁷⁾. Crystal orientation is represented by the Eulerian angle, of which notation is shown in the figure. The SIF varies from that of an isotropic body and the deviation is relatively large at the deepest point rather than it at the surface point. The change in SIF depends on crystal orientation and is not always symmetric. Moreover, the magnitude of change depends on the degree of elastic anisotropy ⁽⁵⁴⁾. Copper exhibited large deviation in SIF from that of an isotropic body, while that of a single tungsten crystal was almost equivalent. It was pointed out that the change in SIF of a surface crack is brought

about by the deformation constraint in a finite body ⁽⁵⁰⁾.

3.2 SIF in polycrystals

In a polycrystalline body, nonuniform stress appears at the microstructural level (local stress) due to random crystallographic and morphologic texture even under a uniform remote stress condition. The difference in local stress is governed primarily by the crystallographic orientation of grains, and is affected by that of neighboring grains, as well. In the vicinity of a grain boundary, the local stress varies due to elastic incompatibility of grains. Such inhomogeneity in local stress in a polycrystalline body can be evaluated by FEA, considering the anisotropic elasticity of each crystal grain and the crystallographic structure of the body ⁽⁵⁸⁾⁻⁽⁶⁵⁾. Once the local stress distribution is evaluated, the influence of inhomogeneous stress on the SIF can be assessed using a numerical method such as the influence function method ⁽⁶⁶⁾, the finite element alternating method ⁽⁶⁷⁾⁻⁽⁶⁹⁾, or the weight function method ⁽⁷⁰⁾. However, it is not easy to identify the morphological structure as well as crystal orientation of each grain in a three-dimensional field. From the practical point of view, the statistical growth behavior of whole cracks is more relevant than the determinate growth of individual cracks, because numerous cracks are initiated in SCC and only some of them contribute to the emergence of macroscopic cracks ⁽⁷¹⁾⁻⁽⁷³⁾. When the crack is sufficiently large, by averaging the changes in SIF at each point along the crack front, statistical changes in SIF due to local stress are negligibly small, although they are significant for a small crack.

Li and Ravichandran ⁽⁷⁰⁾⁽⁷⁴⁾ evaluated the SIF of a semi-elliptical surface crack in a polycrystalline material by a weight function technique. A polycrystalline body was modeled as an ensemble of hexagon-shaped grains with random crystal orientations. The fluctuation in SIF of microstructurally-small-cracks in the polycrystalline body was significant, and was quantified statistically. However, they calculated local stress from the equivalent elastic modulus, which was derived from crystal orientation against the loading direction. Therefore, the influence of constraint between neighboring grains was not taken into account and the stress distribution inside the grain was uniform. The authors also examined the SIF in a polycrystalline body, consisting of hexagonal pillar grains with random crystal orientation, as illustrated in Fig. 14 ⁽⁷⁵⁾. The inhomogeneous local stress as well as the SIF was evaluated by FEA based on a model of a three-dimensional cracked body under remote tensile loading. Then, the influence of the anisotropy of each crystal in addition to local stress was rigorously evaluated in the SIF. In order to represent the variation in SIF, the averaged SIF along the crack front was defined by the following equation:

Fig. 14 Stress intensity factors of semi-circular surface crack in polycrystal of random orientations.

Fig. 15 Variation of normalized SIF during crack growth.

$$F_{\text{lave}} = \frac{1}{\pi a} \int \frac{K_I}{S_o \sqrt{\pi a}} d\Gamma \quad (5)$$

where a is the depth of the crack and Γ denotes the path along the crack front. The standard deviation of the variation in the averaged SIF was quantified as shown in Fig. 14 through 400 calculations of different combinations of crystal orientations. The result revealed that the distribution of the averaged SIF statistically followed the normal distribution and the mean value was the same as that of a crack in an isotropic body. The standard deviation of the averaged SIF decreased as the crack became large and depended on the material properties⁽⁵⁷⁾.

3.3 SIF at grain boundaries

It is known that cracks along interfaces between dissimilar elastic solids often exhibit so-called oscillatory stress field near the tip⁽⁷⁶⁾. Cracks along the boundaries of crystal grains, phases and particle/matrix boundary might have such stress field. For bimetal media consisting of identical orthotropic solids with different crystal orientations on either side, no oscillation presents and the crack tip stress field has the standard square root singularity⁽⁷⁷⁾. It is therefore not necessary to consider the peculiar singularity near the tip of intergranular cracks in orthotropic materials. Statistical investigation of grain boundary cracks in a polycrystalline material revealed that the standard deviation of the variation in SIF was almost the same as that for the transgranular crack shown in Fig. 14⁽⁵⁶⁾.

4. Changes in SIF during crack growth

In order to evaluate the statistical behavior of microstructurally-small-cracks in a polycrystalline body, the authors evaluated the local SIF (K_{local}), which takes into account the influence of the change in crack shape (hereinafter termed “shape effect”) and anisotropy of crystal grain and inhomogeneous local stress distribution (hereinafter termed “polycrystal effect”) as follows⁽⁷⁸⁾:

$$K_{\text{local}} = CF_{\text{poly}} F_{\text{shape}} S_o \sqrt{\pi a} \quad (6)$$

where F_{poly} and F_{shape} represent the magnitudes of the polycrystal effect and shape effect, respectively. C is a constant, a is crack size, and S_0 is the remote applied stress. The magnitude of the polycrystal effect can be determined from the statistical change in SIF, as shown in Fig. 14, which signifies that large cracks are minimally affected by the polycrystal effect. As for the shape effect, when a crack propagates along crack boundaries without bifurcation, the change in SIF due to crack shape can be approximated by Eq.(1) by taking into account the angle of deflection at each crack tip. Since the typical distribution of the angle of deflection along the crack path has been investigated for the intergranular SCC⁽³⁰⁾, it is possible to evaluate the statistical change in SIF due to the kink. Several grains are adjacent to the crack front as shown in Fig. 11(b), and the SIF varies along the crack front corresponding to the shape condition of each grain. Assuming that N_g is the number of grains existing along the crack front, the shape effect can be evaluated by the following equation:

$$F_{\text{shape}} = \frac{\sum_i^{N_g} k_1^{(i)}}{N_g} \frac{1}{CS_0 \sqrt{\pi a}} \quad (7)$$

where $k_1^{(i)}$ is the SIF of the crack tip at the i -th grain. Using the values F_{poly} and F_{shape} obtained, statistical crack growth behavior was estimated using a Monte Carlo simulation by incorporating the empirical relationship between the SIF and crack growth rate⁽⁷⁹⁾. An example of the change in SIF during crack growth is shown in Fig.15, in which grain size is $d = 9.5 \mu\text{m}$. Although fluctuation is large for a small crack, SIF converges for macroscopic cracks ($F_1 = 1.0$) as the crack grows. Thus, the SIF of microstructurally-small-cracks is strongly influenced by crystal grain, possibly resulting in complex processes of growth.

5. Conclusions

In this paper, the influences of crystal grain on the SIF of microstructurally small cracks have been briefly reviewed. Firstly, the SIF of kinked and branched cracks was outlined. It depends on geometrical factors such as the angle of kink and bifurcation. The SIF of a kinked tip can be estimated from the angle of deflection of the grain boundary at the crack tip regardless of the crack shape. Secondly, the SIF of surface crack in an anisotropic body as well as that in an inhomogeneous polycrystalline body was summarized. In particular, statistical changes in SIF were shown as a function of crack size. Finally, based on the results obtained, the statistical changes in SIF and their influences on growth behavior of the microstructurally-small-cracks were discussed. Crystal grain causes fluctuation in the SIF when the crack is microstructurally small, and may induce complex processes of growth.

For accurate prediction of the growth of microstructurally-small-cracks, the SIF should be evaluated based on realistic assumptions of crack shape and stress distribution, rather than simplifications of them⁽⁸⁰⁾⁽⁸¹⁾. The influence of material properties on crack growth is also of key importance, but has not been included in this review.

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