

# Calculation of Stress Intensity Factors and Crack Opening Displacements for Cracks Subjected to Complex Stress Fields

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*Fatigue cracks in shot peened and case hardened notched machine components and high-pressure vessels are subjected to the stress fields induced by the external load and the residual stress resulting from the surface treatment or autofretting. Both stress fields are usually nonuniform and available handbook stress intensity factor solutions are in most cases unavailable for such configurations, especially in the case of two-dimensional surface breaking cracks such as semi-elliptical and quarter-elliptical cracks at notches. The method presented in the paper makes it possible to calculate stress intensity factors for such cracks and complex stress fields by using the generalized weight function technique. It is also shown that the generalized weight functions make it possible to calculate the crack opening displacement field often used in the determination of the critical load or the critical crack size. [DOI: 10.1115/1.1593080]*

## Introduction

Fatigue durability, damage tolerance, and strength evaluations of cracked structural components require calculation of stress intensity factors for cracks subjected to complex stress fields. The variety of crack configurations and the complexity of stress fields occurring in engineering components require more versatile tools for calculating stress intensity factors than available handbook solutions, obtained for a range of specific geometry and load combinations. Therefore, a method for calculating stress intensity factors for cracks subjected to complex stress fields is discussed below. The method is based on the use of the weight function technique.

The application of the weight function technique to the analysis of fatigue crack growth in autofretted high pressure vessels was presented at previous conference [1]. The detail numerical procedure for calculating stress intensity factors and crack opening displacements of cracks subjected to nonlinear stress distributions such as those in autofretted cylinders or near notches is discussed below.

## Stress Intensity Factors and Weight Functions

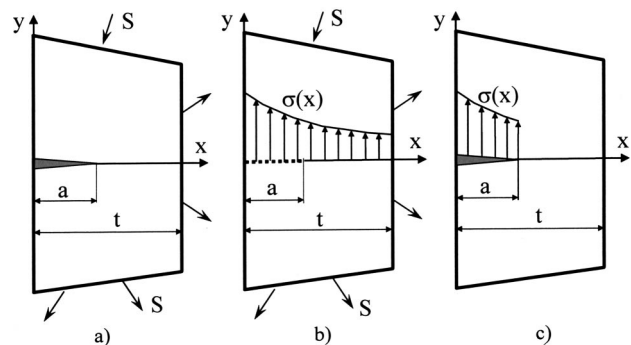
Most of the existing methods of calculating stress intensity factors require separate analysis of each load and geometry configuration. Fortunately, the weight function method developed by Bueckner [2] and Rice [3] simplifies considerably the determination of stress intensity factors. If the weight function is known for a given cracked body, the stress intensity factor due to any load system applied to the body can be determined by using the same weight function. It can be shown [4] that the stress intensity factor for a cracked body (Fig. 1a) subjected to the external loading  $S$  is the same as the stress intensity factor in a geometrically identical body (Fig. 1c) with the local stress field  $\sigma(x)$  applied to the crack faces. The local stress field,  $\sigma(x)$ , induced in the prospective crack plane, is determined for an uncracked body (Fig. 1b) which makes the stress analysis relatively simple. The stress intensity

factor for a one-dimensional crack can be obtained by multiplying the weight function  $m(x,a)$  and the internal stress distribution  $\sigma(x)$  in the prospective crack plane, and integrating the product over the crack length  $a$ ,

$$K = \int_0^a \sigma(x)m(x,a)dx. \quad (1)$$

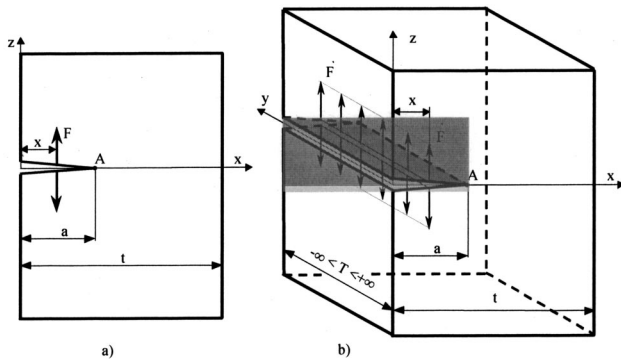
The weight function  $m(x,a)$  can be interpreted (Fig. 2a) as the stress intensity factor that results from a pair of splitting forces,  $F=1$ , applied to the crack face at position  $x$ . The unit force  $F$  shown in Fig. 2a represents actually a uniformly distributed pressure along a line normal to the plane  $xy$  (Fig. 2b).

Since the stress intensity factor is linearly dependent on the applied load, the contributions from multiple splitting forces applied over the crack surface can be superposed and the resultant stress intensity factor can be calculated as the sum of all individual load contributions. This results in the integral, Eq. (1), of the product of the weight function  $m(x,a)$  and the stress function



**Fig. 1** The principle of superposition used in calculation of stress intensity factors based on the weight function technique. **a** Loaded cracked body. **b** The stress distribution in the prospective crack plane. **c** The “uncracked” stress field applied to the crack surface.

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**Fig. 2 Example of the notation and the system of co-ordinates for the weight function: a one-dimensional representation; b interpretation of the point load in three-dimensional bodies**

$\sigma(x)$  for a continuously distributed stress field. A variety of one-dimensional (line-load) weight functions can be found in Refs. [5–7]. However, their mathematical forms vary from case to case and they are not easy to use. Therefore, Glinka and Shen [8] proposed one general weight function expression, which can be used for a wide variety of one-dimensional mode I cracks,

$$m(x,a) = \frac{2F}{\sqrt{2\pi(a-x)}} \left[ 1 + M_1 \left(1 - \frac{x}{a}\right)^{1/2} + M_2 \left(1 - \frac{x}{a}\right)^1 + M_3 \left(1 - \frac{x}{a}\right)^{3/2} \right] \quad (2)$$

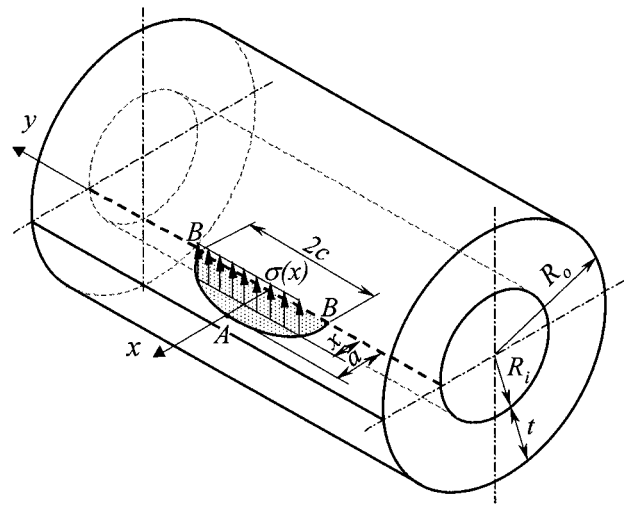
The system of coordinates and the notation for an edge crack as an example are given in Fig. 2. In order to determine the weight function  $m(x,a)$  for a particular cracked body, it is sufficient to determine [9] the three parameters  $M_1$ ,  $M_2$ , and  $M_3$  in expression (2). Because the mathematical form of the weight function (2) is the same for all cracks, the same method can be used for the determination of parameters  $M_1$ ,  $M_2$ , and  $M_3$  and calculation of stress intensity factors from Eq. (1). The method of finding the  $M_i$  parameters was discussed in Ref. [9]. A variety of line load weight functions [8–14] have been derived and published already.

In order to calculate stress intensity factors using the weight function technique the following tasks need to be carried out:

- Determine stress distribution  $\sigma(x)$  in the prospective crack plane using the linear elastic analysis of uncracked body (Fig. 1b), i.e., perform the stress analysis ignoring the crack and determine the stress distribution  $\sigma(x) = \sigma_0 f(S,x)$ .
- Apply the “uncracked” stress distribution,  $\sigma(x)$ , to the crack surfaces (Fig. 1c) as tractions.
- Choose an appropriate generic weight function.
- Integrate the product of the stress function  $\sigma(x)$  and the weight function  $m(x,a)$  over the entire crack length or crack surface, Eq. (1).

### Universal Weight Functions for Two-Dimensional Part-Through Surface and Corner Cracks

In the case of two-dimensional (2D) cracks such as semi-elliptical and corner surface cracks in plates and cylinders the stress intensity factor changes along the crack front. However, in most practical cases the deepest point A (Fig. 3) and the surface point B are associated with the highest and the lowest value of the stress intensity factor along the crack front. Therefore, the weight functions for the point A and B have been derived analogously to the universal weight function (2).



**Fig. 3 Weight function notation for a semi-elliptical crack in a thick-walled cylinder**

- For point A (Fig. 3)

$$m_A(x,a,a/c,a/t) = \frac{2}{\sqrt{2\pi(a-x)}} \left[ 1 + M_{1A} \left(1 - \frac{x}{a}\right)^{1/2} + M_{2A} \left(1 - \frac{x}{a}\right)^1 + M_{3A} \left(1 - \frac{x}{a}\right)^{3/2} \right] \quad (3)$$

- For point B (Fig. 3)

$$m_B(x,a,a/c,a/t) = \frac{2}{\sqrt{\pi x}} \left[ 1 + M_{1B} \left(\frac{x}{a}\right)^{1/2} + M_{2B} \left(\frac{x}{a}\right)^1 + M_{3B} \left(\frac{x}{a}\right)^{3/2} \right] \quad (4)$$

The weight functions  $m_A(x,a)$  and  $m_B(x,a)$  given above and corresponding to the deepest and the surface point A and B respectively have been derived for one-dimensional stress fields (Fig. 3), dependent on one variable  $x$  only. The weight function parameters  $M_{iA}$  and  $M_{iB}$  are given in Ref. [11].

### The Integration Method

One of the difficulties in using the weight function method is accurate integration of the product of the stress function and the weight function as shown in Eq. (1). The stress field  $\sigma(x)$  can be very complex and nonlinear and analytical integration is seldom easy in practice. Also, standard numerical integration methods are inaccurate due to the singularity of the weight function at the crack tip. Therefore, a special integration routine has been developed resulting in highly accurate integration of arbitrary stress functions.

Obtaining an analytical closed form integral (1) might be often difficult or impossible for a nonlinear stress field  $\sigma(x)$  but it is feasible for a linear stress function. Therefore it is very convenient to approximate the stress function as a series of linear segments as shown in Fig. 4. The stress function  $\sigma(x)$  over the linear segment  $i$  can be given in the form of the linear equation (5),

$$\sigma(x) = A_i x + B_i \quad (5)$$

Thus the contribution to the stress intensity factor associated with

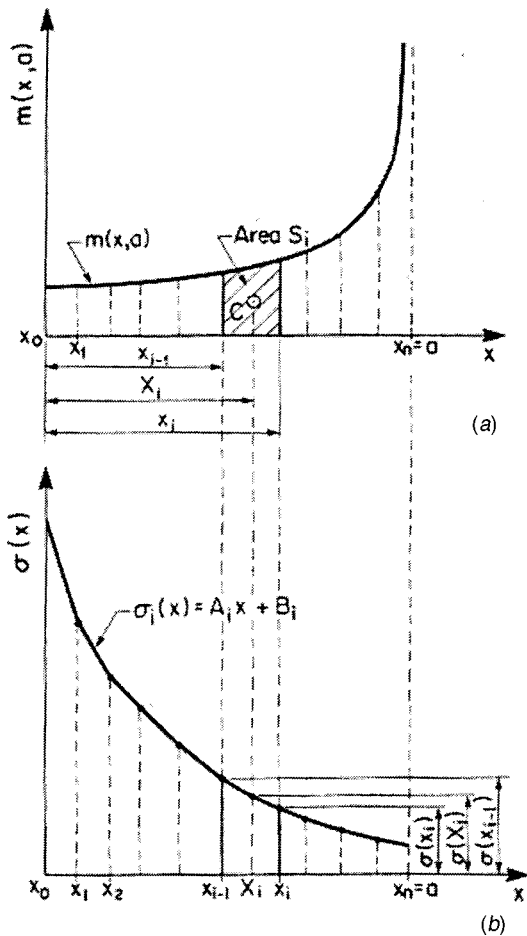


Fig. 4 Application of the simplified integration method: (a) the weight function  $m(x,a)$  and (b) nonlinear stress distribution  $\sigma(x)$

the stress segment  $i$  can be calculated from Eq. (1) after substituting appropriate expressions for the stress and the weight function. The solutions given below have been derived for the deepest and for the surface point of semi-elliptical crack using the weight function (3) and (4), respectively. The solution to one-dimensional cracks is the same as for the deepest point of semi-elliptical cracks.

- Deepest point A (Fig. 4),

$$K_i^A = \int_{x_{i-1}}^{x_i} (A_i x + B_i) \frac{2}{\sqrt{2\pi a \left(1 - \frac{x}{a}\right)}} \times \left[ 1 + M_{1A} \left(1 - \frac{x}{a}\right)^{1/2} + M_{2A} \left(1 - \frac{x}{a}\right)^1 + M_{3A} \left(1 - \frac{x}{a}\right)^{3/2} \right] dx. \quad (6)$$

- Surface point B (Fig. 4),

$$K_i^B = \int_{x_{i-1}}^{x_i} (A_i x + B_i) \frac{2}{\sqrt{2\pi a \left(1 - \frac{x}{a}\right)}} \times \left[ 1 + M_{1B} \left(\frac{x}{a}\right)^{1/2} + M_{2B} \left(\frac{x}{a}\right)^1 + M_{3B} \left(\frac{x}{a}\right)^{3/2} \right] dx. \quad (7)$$

The closed form expressions resulting from the integration of Eqs. (6) and (7) are given below.

- Deepest point A (Fig. 4),

$$K_i^A = \sqrt{\frac{2}{\pi a}} \left[ \alpha_i (C_{i1} + M_{1A} C_{i2} + M_{2A} C_{i3} + M_{3A} C_{i4}) + \beta_i (C_{i3} + M_{1A} C_{i4} + M_{2A} C_{i5} + M_{3A} C_{i6}) \right], \quad (8)$$

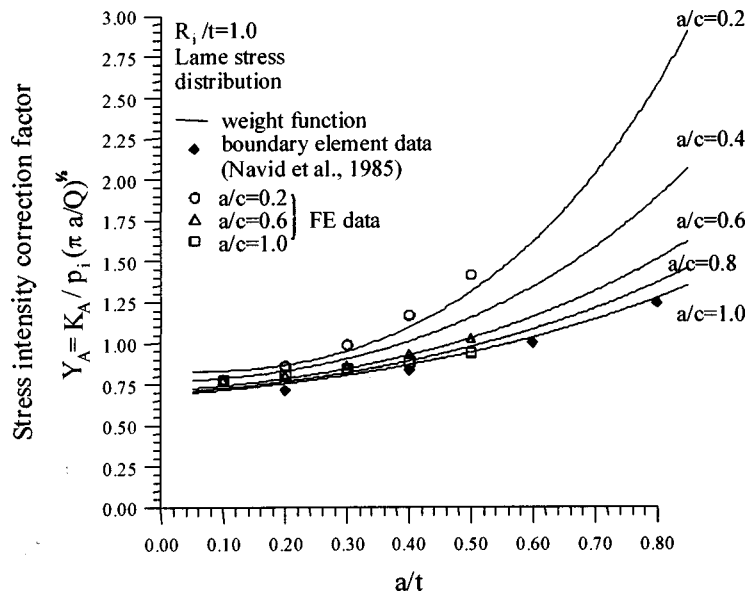


Fig. 5 Comparison of weight function based stress intensity factors for a semi-elliptical internal crack in a pressurized thick-walled cylinder with finite element data

where:

$$\alpha_i = B_i + aA_i \quad \text{and} \quad \beta_i = -aA_i,$$

$$C_{i1} = 2a \left[ \left( 1 - \frac{x_{i-1}}{a} \right)^{1/2} - \left( 1 - \frac{x_i}{a} \right)^{1/2} \right],$$

$$C_{i2} = a \left[ \left( 1 - \frac{x_{i-1}}{a} \right)^1 - \left( 1 - \frac{x_i}{a} \right)^1 \right],$$

$$C_{i3} = \frac{2a}{3} \left[ \left( 1 - \frac{x_{i-1}}{a} \right)^{3/2} - \left( 1 - \frac{x_i}{a} \right)^{3/2} \right],$$

$$C_{i4} = \frac{a}{2} \left[ \left( 1 - \frac{x_{i-1}}{a} \right)^2 - \left( 1 - \frac{x_i}{a} \right)^2 \right],$$

$$C_{i5} = \frac{2a}{5} \left[ \left( 1 - \frac{x_{i-1}}{a} \right)^{5/2} - \left( 1 - \frac{x_i}{a} \right)^{5/2} \right],$$

$$C_{i6} = \frac{a}{3} \left[ \left( 1 - \frac{x_{i-1}}{a} \right)^3 - \left( 1 - \frac{x_i}{a} \right)^3 \right].$$

Surface point B (Fig. 4),

$$K_i^B = \frac{2}{\sqrt{\pi a}} \begin{bmatrix} (\alpha_i + \beta_i) \times \\ (D_{i1} + M_{1B}D_{i2}) \\ (+ M_{2B}D_{i3} + M_{3B}D_{i4}) \\ -\beta_i (D_{i5} + M_{1B}D_{i6}) \\ (+ M_{2B}D_{i5} + M_{3B}D_{i6}) \end{bmatrix}, \quad (9)$$

where

$$\alpha_i = B_i + aA_i \quad \text{and} \quad \beta_i = -aA_i,$$

$$D_{i1} = 2a \left[ \left( \frac{x_i}{a} \right)^{1/2} - \left( \frac{x_{i-1}}{a} \right)^{1/2} \right]; \quad D_{i2} = a \left[ \left( \frac{x_i}{a} \right)^1 - \left( \frac{x_{i-1}}{a} \right)^1 \right],$$

$$D_{i3} = \frac{2a}{3} \left[ \left( \frac{x_i}{a} \right)^{3/2} - \left( \frac{x_{i-1}}{a} \right)^{3/2} \right]; \quad D_{i4} = \frac{a}{2} \left[ \left( \frac{x_i}{a} \right)^2 - \left( \frac{x_{i-1}}{a} \right)^2 \right],$$

$$D_{i5} = \frac{2a}{5} \left[ \left( \frac{x_i}{a} \right)^{5/2} - \left( \frac{x_{i-1}}{a} \right)^{5/2} \right]; \quad D_{i6} = \frac{a}{3} \left[ \left( \frac{x_i}{a} \right)^3 - \left( \frac{x_{i-1}}{a} \right)^3 \right],$$

$$\alpha_i = B_i + aA_i \quad \text{and} \quad \beta_i = -aA_i,$$

$$D_{i1} = 2a \left[ \left( \frac{x_i}{a} \right)^{1/2} - \left( \frac{x_{i-1}}{a} \right)^{1/2} \right]; \quad D_{i2} = a \left[ \left( \frac{x_i}{a} \right)^1 - \left( \frac{x_{i-1}}{a} \right)^1 \right],$$

$$D_{i3} = \frac{2a}{3} \left[ \left( \frac{x_i}{a} \right)^{3/2} - \left( \frac{x_{i-1}}{a} \right)^{3/2} \right]; \quad D_{i4} = \frac{a}{2} \left[ \left( \frac{x_i}{a} \right)^2 - \left( \frac{x_{i-1}}{a} \right)^2 \right],$$

$$D_{i5} = \frac{2a}{5} \left[ \left( \frac{x_i}{a} \right)^{5/2} - \left( \frac{x_{i-1}}{a} \right)^{5/2} \right]; \quad D_{i6} = \frac{a}{3} \left[ \left( \frac{x_i}{a} \right)^3 - \left( \frac{x_{i-1}}{a} \right)^3 \right].$$

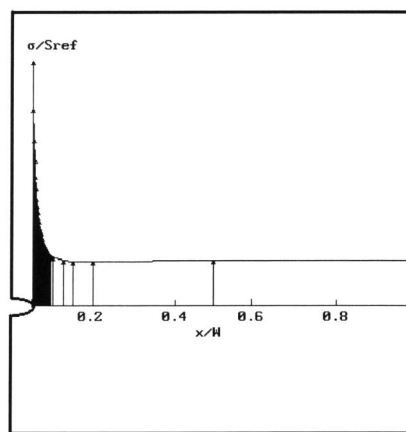
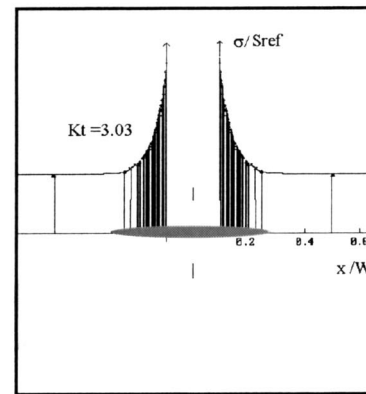
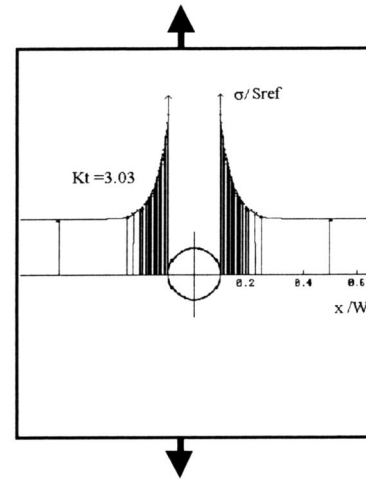
Equations (8) and (9) can be used for calculating stress intensity contributions due to each linear piece of the stress distribution function by substituting appropriate values for  $a$ ,  $x_{i-1}$ ,  $x_i$ ,  $A_i$ , and  $B_i$ . The stress intensity factor  $K$  is finally calculated as the sum of all contributions  $K_i$  from all linear stress segments within the range of  $0 \leq x \leq a$ ,

$$K = \sum_1^n K_i. \quad (10)$$

Thus the integration can be reduced to the substitution of appropriate parameters into Eqs. (8) and (9) and summation according to Eq. (10). This makes it possible to develop a very efficient and accurate numerical integration routine, which is important in the case of lengthy fatigue crack growth analyses.

## Stress Intensity Factors for the Lamé Stress Distribution

The method described above was applied for calculating stress intensity factors due to the Lamé stress distribution applied to a semi-elliptical crack (Fig. 3) in a thick wall cylinder ( $R_i/t=1$ ). The results (Fig. 5) are presented in the form of the geometrical correction factor  $Y_A = K_A/p_i\sqrt{(\pi a/Q)}$ , corresponding to the deepest point A, where  $Q$  is the elliptical integral of the second kind



Name: QHEDGE  
Points: 38

x/W	σ/Sref
0.000	0.000
0.025	0.000
0.050	0.000
0.050	5.220
0.051	4.202
0.053	3.552
0.054	3.100
0.056	2.768
0.058	2.513
0.059	2.311
0.061	2.146

Fig. 6 (a) Modeling the notch and cracks for the use of the weight function method, and (b) Stress distribution ahead of a semi-elliptical edge notch in a wide plate under uniform tension

Central Circular Hole:  $r=8$  and  $W=80$

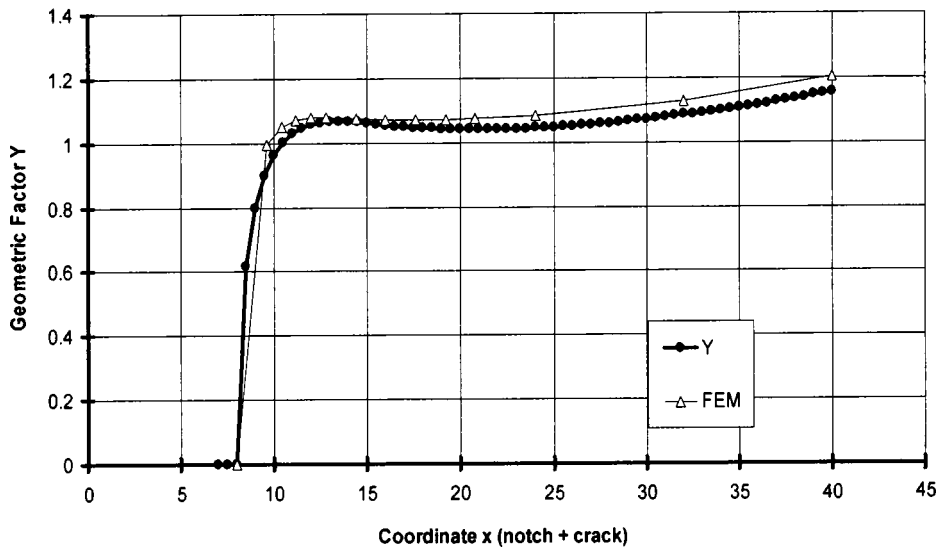


Fig. 7 Stress intensity factor for symmetric cracks emanating from a circular notch in a wide plate

approximated by expression  $Q=1+1.464(a/c)^{1.65}$ . The weight function stress intensity factors agree well with the ASME and finite element data. However, the weight function enables the calculation of stress intensity factors beyond the ASME range of applications, i.e., also for deep cracks with the relative depth of  $a/t > 0.5$ .

The weight functions for cracks in plates can also be used for calculating stress intensity factors for cracks emanating from notches (Figs. 6 and 7). The notch and the actual crack are treated as one crack but loaded only over the region coincided with depth of the actual crack. The stress distribution (Figs. 6–8) is that, which would exist near the notch tip in the absence of the crack. The weight function based stress intensity factors agree reasonably well with the finite element data [15]—see Figs. 7 and 8. The geometrical  $Y$  factors presented in Figs. 7 and 8 are defined as  $Y=K/S\sqrt{\pi a}$ , where  $S$  is the nominal remote stress in the gross section.

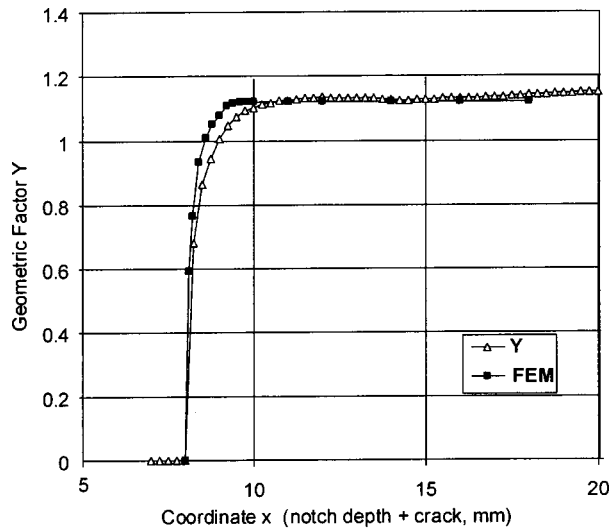


Fig. 8 Stress intensity factors for cracks emanating from a semi-elliptical edge notch in a wide plate (depth  $d=8$ , notch radius  $r=2$ , plate width  $W=160$ )

Crack Opening Displacements

The weight function and the stress intensity factor are uniquely related to the crack opening displacement field which can be obtained by integrating the stress intensity factor and the weight function,

$$m(x,a) = \frac{E'}{K(a)} \frac{\partial u(x,a)}{\partial a} \quad (11)$$

If the stress intensity factor  $K(a)$  induced by the stress distribution  $\sigma(x)$  is known then the crack opening displacement at any coordinate  $x$  can be determined,

$$u(x,a) = \frac{1}{E'} \int_x^a K(\alpha)m(x,\alpha)d\alpha \quad (12)$$

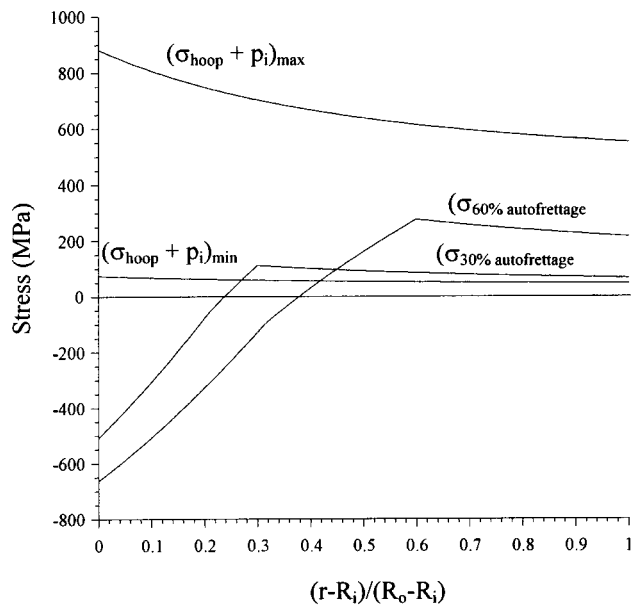
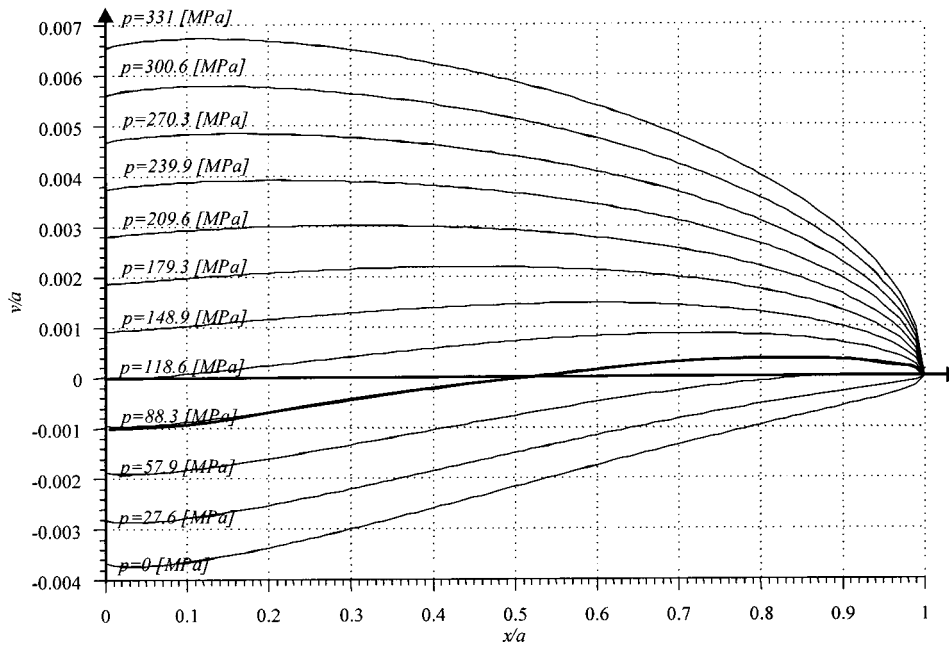


Fig. 9 The hoop and residual stress distribution in a thick wall cylinder under internal pressure  $p_i$



**Fig. 10** Opening displacements of an internal edge crack in autofrettaged thick-walled cylinder subjected to internal pressure  $p_i$

Substitution of expression (1) into Eq. (12) results in the final relationship enabling the crack opening displacement to be calculated based on the weight function and the stress field applied to the crack surface,

$$u(x, a) = \frac{1}{E'} \int_x^a [\sigma(x') m(x, \alpha) dx'] m(x, \alpha) d\alpha. \quad (13)$$

In some cases closed form solutions are attainable but most often numerical techniques have to be employed for calculating the integral of Eq. (13). Substitution of the general weight function (2) into the above formulas results in the expression (14),

$$u(x, a) = \frac{1}{E'} \sqrt{\frac{2}{\pi}} \int_x^a \frac{K_1(\alpha)}{\sqrt{\alpha-x}} \left[ 1 + M_1 \left( 1 - \frac{x}{\alpha} \right)^{1/2} + M_2 \left( 1 - \frac{x}{\alpha} \right) + M_3 \left( 1 - \frac{x}{\alpha} \right)^{3/2} \right] d\alpha, \quad (14)$$

where  $K_1(\alpha)$  is determined for a crack with an instantaneous length of  $\alpha$ ,

$$K_1(\alpha) = \sqrt{\frac{2}{\pi}} \int_0^\alpha \frac{\sigma(x)}{\sqrt{\alpha-x}} \left[ 1 + M_1 \left( 1 - \frac{x}{\alpha} \right)^{1/2} + M_2 \left( 1 - \frac{x}{\alpha} \right) + M_3 \left( 1 - \frac{x}{\alpha} \right)^{3/2} \right] dx. \quad (15)$$

The stress intensity  $K_1(\alpha)$  for the instantaneous crack length  $\alpha$  can be calculated using the method describe above.

With the exception of cracks in infinite or semi-infinite bodies, the parameters,  $M_i$  ( $i=1,2,3$ ), of the general weight function are continuous but usually are nonstandard functions of the ratio of a crack length to the characteristic dimension of the body, such as a plate width. Also, the stress intensity factor  $K_1(\alpha)$  for an arbitrary stress distribution may become a complicated function of the crack length. Therefore, in general, calculation of crack surface displacements using the integral relationships above must be performed numerically.

The integral in Eq. (14) contains the term  $1/(a-x)^{1/2}$  that becomes singular at one end of the integration interval. A specialized

Gaussian quadrature technique for evaluating integrals with such a singular term was adopted to calculate crack surface displacements.

Several theoretical studies have been carried out concerning the profile of an opened crack subjected to complex stress fields. Among them an edge crack in a thick-wall cylinder subjected to nonlinear residual and the Lamé stress has been analyzed. An example of the resultant stress fields is shown in Fig. 9. The opened crack profiles corresponding to several pressure levels are presented in Fig. 10. As discussed in Ref. [1] a crack may first close at the mouth rather than at the tip, as pressure is reduced.

## Conclusions

A method of calculating stress intensity factors for cracks subjected to complex stress fields has been discussed in the paper. The method is based on the use of generalized weight functions. It has been shown that the weight functions enable the determination of stress intensity factors for a variety of geometrical and stress field configurations. The crack opening displacement analysis based also on the use of the same weight functions revealed that crack in autofrettaged cylinder may remain partially closed indicating that the usual superposition method might not be valid in some cases.

## References

- [1] Kiciak, A., Burns, D. J., and Glinka, G., 2001, "Effects of mouth closure and fluid entrapment on fatigue crack propagation in thick-walled autofrettaged cylinders," *ASME Pressure Vessel Conference, PVP*, Vol. 418, pp. 19–30.
- [2] Bueckner, H. F., 1970, "A novel principle for the computation of stress intensity factors," *Z. Angew. Math. Mech.*, **50**, pp. 529–546.
- [3] Rice, J. R., 1972, "Some remarks on elastic crack-tip stress field," *Int. J. Solids Struct.*, **8**, pp. 751–758.
- [4] Broek, D., 1988, *The Practical Use of Fracture Mechanics*, Kluwer, Amsterdam.
- [5] Tada, H., Paris, P., and Irwin, G., 1985, *The Stress Analysis of Cracks Handbook*, 2nd Edn. Paris Production Inc., St. Louis, Missouri, USA.
- [6] Wu, X. R., and Carlsson, A. J., 1991, *Weight Functions and Stress Intensity Factor Solutions*, Pergamon Press, Oxford, UK.
- [7] Fett, T., and Munz, D., 1994, *Stress Intensity Factors and Weight Functions for One-dimensional Cracks*, Report No. KfK 5290, Kernforschungszentrum Karlsruhe, Institut für Materialforschung, Karlsruhe, Germany.
- [8] Glinka, G., and Shen, G., 1991, "Universal features of weight functions for cracks in mode I," *Eng. Fract. Mech.*, **40**, pp. 1135–1146.

- [9] Shen, G., and Glinka, G., 1991, "Determination of weight functions from reference stress intensity factors," *Theor. Appl. Fract. Mech.*, **15**, pp. 237–245.
- [10] Shen, G., and Glinka, G., 1991, "Weight functions for a surface semi-elliptical crack in a finite thickness plate," *Theor. Appl. Fract. Mech.*, **15**, pp. 247–255.
- [11] Zheng, X. J., Glinka, G., and Dubey, R., 1995, "Calculation of stress intensity factors for semi-elliptical cracks in a thick-wall cylinder," *Int. J. pressure vessels piping*, **62**, pp. 249–258.
- [12] Zheng, X. J., Glinka, G., and Dubey, R., 1996, "Stress intensity factors and weight functions for a corner crack in a finite thickness plate," *Eng. Fract. Mech.*, **54**, pp. 49–62.
- [13] Wang, X., and Lambert, S. B., 1995, "Stress intensity factors for low aspect ratio semi-elliptical surface cracks in finite-thickness plates subjected to non-uniform stresses," *Eng. Fract. Mech.*, **51**, pp. 517–532.
- [14] Wang, X., and Lambert, S. B., 1997, "Stress intensity factors and weight functions for high aspects ratio semi-elliptical surface cracks in finite-thickness plates," *Eng. Fract. Mech.*, **57**, pp. 13–24.
- [15] Kitagawa, H., and Yuuki, R., 1977, "Analysis of the non-linear shaped cracks in a finite plate by the conformal mapping method," *Trans. Jpn. Soc. Mech. Eng.*, **43**, pp. 4354–4362.