6 RATES OF ENERGY RELEASE RATE FOR AND STABILITY OF A 3D PLANAR CRACK OF ARBITRARY SHAPE

The derivatives of energy release rates are important parameters in some fracture mechanics problems. In Section 5, equations for the prediction of stability and arrest of a single crack, and the growth pattern of a system of interacting cracks were presented. Another important LEFM problem is shape prediction (Bui, 1979; Souza, 1992; Nguyen, 1980, 1994) and stability analysis (Rice, 1985; Gao, 1986, 1987a, 1987b, 1989; Nguyen, 1980, 1990, 1994) of an evolving 3D crack.

For example, the first order variation of energy release rate, and thus the second variation of potential energy with respect to local crack extension, is required to study the stability of a planar crack of arbitrary shape. The second variation can be used to predict the shape of a propagating crack, using a concept of maximization of total energy released as a crack propagates in brittle fracture. Also, the second variation is necessary to investigate configurational stability versus small deviations from the fundamental shape of an evolving crack front in fatigue crack propagation. Therefore, an important requirement of some fracture mechanics analyses is to evaluate accurately the energy release rates and their higher order derivatives for a body containing a 3D planar crack of arbitrary shape, subjected to arbitrary loadings, including crack-face loading, thermal loading and body forces.

There have been several numerical methods for calculating the derivatives of energy release rates. De Koning *et al.* (1984) calculated the derivatives of crack-opening displacement and stress intensity factor due to virtual crack front perturbations for a three-dimensional planar crack of arbitrary shape, based on finite elements and stiffness derivative technique. In their approach, finite perturbations of finite element meshes are applied to approximate the stiffness derivative by subtracting two stiffness matrices.

Meade and Keer (1984a, b) analyzed the half-plane crack with a slightly wavy crack front subjected to mode-I loading using asymptotic expansion and presented the first order variation of stress intensity factor due to variation in crack geometry. Rice (1985) developed, using three-dimensional weight function theory, a linear perturbation scheme for calculating the first order variation in stress intensity factor and crack opening displacement due to small changes in three-dimensional planar crack geometry. Nguyen *et al.* (1990) introduced an explicit expression for the matrix of the second derivatives of energy with respect to the crack lengths in terms of path-independent integrals. Destyunder *et al*. (1983) introduced a geometrical Lagrangian description to derive the expression for the energy release rates in terms of Lagrangian variables. Bonnet (1994) extended the concepts of shape differentiation of Destyunder *et al.* to develop a Galerkin-type symmetric boundary integral equation formulation for the energy release rates and their rates around an arbitrary shaped crack.

In this Section, the variational formulation for the derivatives of energy release rates presented in Section 5 is extended to the problems of a 3D crack with an arbitrarily curved front. The method provides the direct integral forms of stiffness derivatives, and thus there is no need for the analyst to specify a finite length of virtual crack extension. The salient feature of this method is that the energy release rates and their higher derivatives for three-dimensional cracks of arbitrary shape can be computed in a single analysis. Furthermore, the generalized formulation for the 3D crack problem has a couple of new features. First, the method considers the interaction between virtual crack extensions at different positions along the crack front, because the areas perturbed due to crack extensions at adjacent positions on the front are overlapped. The additional term representing the interaction between virtual crack extensions is explicitly derived and included in the formulation for the second variations of element stiffness. Secondly, it is shown that a local curvature on the curved crack front must be taken into account to properly calculate the derivatives of energy release rate. The general formula for the derivatives of energy release rates around an arbitrarily curved front is provided.

In Section 6.1, the explicit expressions for energy release rate and its rates are derived for a three-dimensional crack with arbitrarily curved front under arbitrary loading. The details of the general formulation are described, including the issues of interaction between virtual crack extensions and the effect of local crack front curvature on the solution. In section 6.2, several 3-D numerical examples with exact solutions or with solutions available in the literature are solved to demonstrate the accuracy of the current method. These examples include an embedded penny-shaped crack in a large cylinder under remote uniform tensile loading, a semi-circular surface crack in a half circular cylinder under remote uniform tensile loading, a center cracked plate under remote uniform tensile loading, and a single edge cracked plate under remote uniform tensile loading.

6.1 Formulation

In this section, the explicit expressions for energy release rate and its rates are derived for a three-dimensional crack with curved-front under arbitrary loading. For all the developments reported herein, it is assumed that the crack front will be surrounded by a uniform set of 15-noded wedge elements or 20-noded brick elements with quarter-point nodes, like those described in Section 2, and as shown in Figure 65.

The potential energy Π of a 3-D solid is given by

$$\Pi = \frac{1}{2} u^T K u - u^T f \tag{267}$$

where u, K and f are the nodal displacement vector, the structural stiffness matrix and the applied nodal force vector, respectively. The potential energy change due to a virtual crack front perturbation along the arbitrary crack front can be written as,

$$-\delta\Pi = \int_{\substack{Crack\\Front}} G(s)\,\delta a(s)\,ds = -\frac{1}{2}u^T \delta K\, u + u^T \delta f \qquad (268)$$

where $\delta\Pi$ is the variation in potential energy for a virtual crack extension, $\delta a(s)$ is the local crack front advance in a direction normal to the original crack front and a function of distance s along the crack front, $G(s)$ is the local energy release rate due to $\delta a(s)$, ds denotes an increment of arc length along the crack front, and δK and δf are variations of the structural stiffness matrix and load vector due to virtual crack front advance, respectively.

According to deLorenzi (1982), it is possible to define both local and average values of energy release rate along the crack front. The average energy release rate can be found by advancing all node points on the crack front a distance and dividing the total released energy by the area of the virtual crack extension. The local energy release rate can be evaluated by advancing one node at a time and calculating the area of the virtual crack extension from the finite element interpolation functions, Figure 66.

To calculate the local energy release rate along the crack front, various types of virtual crack extensions are possible, as shown in Figure 67. Banks-Sills (1991) showed that most accurate results are obtained if $\delta a(s)$ varies linearly with crack front arc length for the crack extension (see Figure 67a). In this study, linear virtual crack extension is used. An area perturbed due to virtual crack extension at a point i along the front can be written as,

$$\delta A_i = \int_0^{L_i} \delta a(s)\,ds = \delta a_i\, l_i \qquad (269)$$

where δA_i is a perturbed area, δa_i is the magnitude of virtual crack extension, L_i is the length of the crack front segment and l_i is an effective width of the perturbed area. It seems reasonable to assume that for small enough segments of crack front, the variation of $G(s)$ may be neglected within each crack front segment. Thus, equation (267) can be rewritten as

$$-\delta\Pi = \int_{\substack{Crack\\Front\\Segment}} G(s)\,\delta a(s)\,ds = G_{Average} \int_{\substack{Crack\\Front\\Segment}} \delta a(s)\,ds = G_{Average} \cdot \delta A = G_{Average} \cdot \delta a \cdot l \qquad (270)$$

where $G_{Average}$ is the average energy release rate within a small segment of crack front.

Thus, a local energy release rate due to a virtual crack front perturbation, δA_i, at a point i on the arbitrary crack front can be expressed as,

$$G_i = -\frac{\delta\Pi}{\delta A_i} = -\frac{\delta\Pi}{\delta a_i l_i} \qquad (271)$$

$$G_i = -\frac{\delta\Pi}{\delta A_i} = -\frac{\delta\Pi}{\delta a_i\, l_i} = \frac{1}{l_i}\left(-\frac{1}{2}u^T \frac{\delta K}{\delta a_i}u + u^T \frac{\delta f}{\delta a_i}\right) \qquad (272)$$

It is noted that nonzero contributions to $\delta K / \delta a_i$ and $\delta f / \delta a_i$ occur only over elements perturbed by virtual crack extension. Whenever crack-face, thermal and body force loadings are applied, the variations of loading must be taken into account to reflect the local load change on the crack-face or in the crack tip vicinity as a result of virtual crack extension.

The second order variation of potential energy with respect to the virtual crack extensions at different points, *i* and *j*, on the arbitrary crack front is,

$$-\frac{\delta^2\Pi_i}{\delta a_i \delta a_j} = -u^T \frac{\delta K}{\delta a_i}\frac{\delta u}{\delta a_j} - \frac{1}{2}u^T \frac{\delta^2 K}{\delta a_i \delta a_j}u + \frac{\delta u}{\delta a_j}^T \frac{\delta f}{\delta a_i} + u^T \frac{\delta^2 f}{\delta a_i \delta a_j} \qquad (273)$$

The variation of the displacement is obtained from the variation of the global equilibrium equation $Ku = f$ with respect to a_j,

$$\frac{\delta K}{\delta a_j} u + K \frac{\delta u}{\delta a_j} = \frac{\delta f}{\delta a_j} \quad \text{or} \quad \frac{\delta u}{\delta a_j} = K^{-1}\left(\frac{\delta f}{\delta a_j} - \frac{\delta K}{\delta a_j} u \right) \tag{274}$$

By substituting equation (274) into equation (273), we obtain the final expression

$$\begin{aligned} -\frac{\delta^2 \Pi}{\delta a_i \delta a_j} &= -\frac{1}{2} u^T \frac{\delta^2 K}{\delta a_i \delta a_j} u + u^T \frac{\delta^2 f}{\delta a_i \delta a_j} \\ & -u^T \frac{\delta K}{\delta a_i} K^{-1}\left(\frac{\delta f}{\delta a_j} - \frac{\delta K}{\delta a_j} u \right) + \left(\frac{\delta f}{\delta a_j} - \frac{\delta K}{\delta a_j} u \right)^T K^{-1T} \frac{\delta f}{\delta a_i} \end{aligned} \tag{275}$$

6.1.1 First order derivatives of energy release rates for a crack with arbitrarily curved front

Now, energy release rates and their derivatives for a crack with arbitrarily curved front are derived. Consider a segment of curved crack front with a local radius *R(s)* on the crack front, Figure 68. It is assumed that for small enough segments of crack front, the variation of *R(s)* is neglected within each crack front segment. The area of a circular sector containing the crack front segment is

$$A_i = \frac{1}{2} R_i^{\,2} \theta_i = \frac{1}{2} a_i^{\,2} \theta \quad \text{where } a_i = R_i \tag{276}$$

and its variation due to a small change in radius is given by

$$\delta A_i = \frac{1}{2} R_i \theta_i \, \delta R_i = \delta R_i l_i = \delta a_i l_i \quad \text{for linear perturbation in Figure 67a} \tag{277}$$

$$l_i = \frac{1}{2} R_i \theta_i \tag{278}$$

where A_i is the area of a circular sector influenced by virtual crack front perturbation at crack front node i, R_i is a local radius of curvature at crack front node i, δA_i is the variation of the area A_i due to virtual crack front perturbation, δR_i is the variation of radius and θ_i is the angle of the circular sector.

Thus, energy release rate is given by

$$G_i = -\frac{\delta \Pi}{\delta A_i} = -\frac{\delta \Pi}{\delta R_i}\frac{2}{R_i \theta_i} = -\frac{\delta \Pi}{\delta R_i}\frac{1}{l_i} \tag{279}$$

The rate of energy release rate is

$$\frac{\delta G_i}{\delta R_j} = -\frac{\delta^2 \Pi}{\delta R_i \delta R_j}\frac{2}{R_i \theta_i} + \frac{\delta \Pi}{\delta R_i}\frac{2}{{R_i}^2 \theta_i}\frac{\delta R_i}{\delta R_j} = -\frac{\delta^2 \Pi}{\delta R_i \delta R_j}\frac{1}{l_i} - \frac{G_i}{R_i}\frac{\delta R_i}{\delta R_j} \tag{280}$$

where it is clearly shown that a local curvature on a curved crack front plays an important role in the calculation of rates of energy release rate.

$$\frac{\delta G_i}{\delta a_j} l_i = -\frac{\delta^2 \Pi}{\delta a_i \delta a_j} - \frac{G_i l_i}{R_i}\frac{\delta R_i}{\delta R_j} = -\frac{\delta^2 \Pi}{\delta a_i \delta a_j} - \frac{G_i l_i}{R_i}\delta_{ij} \tag{281}$$

where $\delta R_i / \delta R_j$ is replaced by Kronecker delta δ_{ij} which is 1 for $i = j$ and zero for $i \neq j$ .Thus, the explicit forms of energy release rates and their rates for the general case of a planar crack with an arbitrarily curved front are given by,

$$G_i l_i = -\frac{\delta \Pi}{\delta a_i} = -\frac{1}{2}u^T \frac{\delta K}{\delta a_i} u + u^T \frac{\delta f}{\delta a_i} \tag{282}$$

$$\frac{\delta G_i}{\delta a_j} l_i = -\frac{1}{2}u^T \frac{\delta^2 K}{\delta a_i \delta a_j} u + u^T \frac{\delta^2 f}{\delta a_i \delta a_j}$$
$$-u^T \frac{\delta K}{\delta a_i} K^{-1}\left(\frac{\delta f}{\delta a_j} - \frac{\delta K}{\delta a_j}u\right) + \left(\frac{\delta f}{\delta a_j} - \frac{\delta K}{\delta a_j}u\right)^T K^{-1T}\frac{\delta f}{\delta a_i}$$

$$+\left(\frac{1}{2}u^T\frac{\delta K}{\delta a_i}u-u^T\frac{\delta f}{\delta a_i}\right)\frac{\delta_{ij}}{R_i} \tag{283}$$

6.1.2 Derivations of stiffness derivatives for 3D finite elements

This section provides derivations for stiffness variations of 3D finite elements. Firstly, a strain-like matrix, $\tilde{\varepsilon}$, for the 3-D problem is defined as,

$$\tilde{\varepsilon} = J^{-1}\begin{Bmatrix}\frac{\partial N}{\partial \xi^1}\\ \frac{\partial N}{\partial \xi^2}\\ \frac{\partial N}{\partial \xi^3}\end{Bmatrix}\lfloor \Delta_n^1 \quad \Delta_n^2 \quad \Delta_n^3 \rfloor = \begin{bmatrix} J_{11} & J_{12} & J_{13}\\ J_{21} & J_{22} & J_{23}\\ J_{31} & J_{32} & J_{33}\end{bmatrix}^{-1}\begin{Bmatrix}\frac{\partial N}{\partial \xi^1}\\ \frac{\partial N}{\partial \xi^2}\\ \frac{\partial N}{\partial \xi^3}\end{Bmatrix}\lfloor \Delta_n^1 \quad \Delta_n^2 \quad \Delta_n^3 \rfloor \tag{284}$$

$$\tilde{\varepsilon} = \begin{bmatrix} \tilde{\varepsilon}_{11} & \tilde{\varepsilon}_{12} & \tilde{\varepsilon}_{13}\\ \tilde{\varepsilon}_{21} & \tilde{\varepsilon}_{22} & \tilde{\varepsilon}_{23}\\ \tilde{\varepsilon}_{31} & \tilde{\varepsilon}_{32} & \varepsilon_{33}\end{bmatrix} = \begin{bmatrix}\lfloor \tilde{\varepsilon}_1 \rfloor\\ \lfloor \tilde{\varepsilon}_2 \rfloor\\ \lfloor \tilde{\varepsilon}_3 \rfloor\end{bmatrix} \tag{285}$$

where Δ_n are nodal values of the infinitesimal mesh perturbations Δ. $\tilde{\varepsilon}$ is a strain-like matrix created by the geometry changes of the meshes $\Delta' s$ on the unstrained structure, Figure 69. The strain-displacement matrix, B, for a 3-D problem is

$$B = \begin{bmatrix} \frac{\partial N}{\partial x^1} & & \\ & \frac{\partial N}{\partial x^2} & \\ & & \frac{\partial N}{\partial x^3} \\ \frac{\partial N}{\partial x^2} & \frac{\partial N}{\partial x^1} & \\ & \frac{\partial N}{\partial x^3} & \frac{\partial N}{\partial x^2} \\ \frac{\partial N}{\partial x^3} & & \frac{\partial N}{\partial x^1} \end{bmatrix} \qquad (286)$$

The first order variation of B due to virtual crack extension, δa_i, at a point i on a crack front is defined as

$$\frac{\delta B}{\delta a_i} = -\begin{bmatrix} \lfloor\tilde{\varepsilon}_1\rfloor & & \\ & \lfloor\tilde{\varepsilon}_2\rfloor & \\ & & \lfloor\tilde{\varepsilon}_3\rfloor \\ \lfloor\tilde{\varepsilon}_2\rfloor & \lfloor\tilde{\varepsilon}_1\rfloor & \\ & \lfloor\tilde{\varepsilon}_3\rfloor & \lfloor\tilde{\varepsilon}_2\rfloor \\ \lfloor\tilde{\varepsilon}_3\rfloor & & \lfloor\tilde{\varepsilon}_1\rfloor \end{bmatrix} \begin{bmatrix} \frac{\partial N}{\partial x^1} & & \\ \frac{\partial N}{\partial x^2} & & \\ \frac{\partial N}{\partial x^3} & & \\ & \frac{\partial N}{\partial x^1} & \\ & \frac{\partial N}{\partial x^2} & \\ & \frac{\partial N}{\partial x^3} & \\ & & \frac{\partial N}{\partial x^1} \\ & & \frac{\partial N}{\partial x^2} \\ & & \frac{\partial N}{\partial x^3} \end{bmatrix} \qquad (287)$$

where $\lfloor\tilde{\varepsilon}_1\rfloor$, $\lfloor\tilde{\varepsilon}_2\rfloor$ and $\lfloor\tilde{\varepsilon}_3\rfloor$ are the component matrices of $[\tilde{\varepsilon}]$ defined by

$$\tilde{\varepsilon} = \begin{Bmatrix} \lfloor \tilde{\varepsilon}_1 \rfloor \\ \lfloor \tilde{\varepsilon}_2 \rfloor \\ \lfloor \tilde{\varepsilon}_3 \rfloor \end{Bmatrix} \tag{288}$$

The second order variation of B due to virtual crack extension, δa_i, at a point i on a crack front is written as

$$\frac{\delta^2 B}{\delta a_i^2} = -\begin{bmatrix} \lfloor \tilde{\varepsilon}_1" \rfloor & & \\ & \lfloor \tilde{\varepsilon}_2" \rfloor & \\ & & \lfloor \tilde{\varepsilon}_3" \rfloor \\ \lfloor \tilde{\varepsilon}_2" \rfloor & \lfloor \tilde{\varepsilon}_1" \rfloor & \\ & \lfloor \tilde{\varepsilon}_3" \rfloor & \lfloor \tilde{\varepsilon}_2" \rfloor \\ \lfloor \tilde{\varepsilon}_3" \rfloor & & \lfloor \tilde{\varepsilon}_1" \rfloor \end{bmatrix} \begin{bmatrix} \frac{\partial N}{\partial x^1} & & \\ \frac{\partial N}{\partial x^2} & & \\ \frac{\partial N}{\partial x^3} & & \\ & \frac{\partial N}{\partial x^1} & \\ & \frac{\partial N}{\partial x^2} & \\ & \frac{\partial N}{\partial x^3} & \\ & & \frac{\partial N}{\partial x^1} \\ & & \frac{\partial N}{\partial x^2} \\ & & \frac{\partial N}{\partial x^3} \end{bmatrix} \tag{289}$$

in which $\lfloor \tilde{\varepsilon}_1" \rfloor$, $\lfloor \tilde{\varepsilon}_2" \rfloor$ and $\lfloor \tilde{\varepsilon}_3" \rfloor$ are the component matrices of $[\tilde{\varepsilon}"]$ defined by

$$\tilde{\varepsilon}" = 2\tilde{\varepsilon}^2 = \begin{Bmatrix} \lfloor \tilde{\varepsilon}_1" \rfloor \\ \lfloor \tilde{\varepsilon}_2" \rfloor \\ \lfloor \tilde{\varepsilon}_3" \rfloor \end{Bmatrix} = 2\begin{bmatrix} \tilde{\varepsilon}_{11} & \tilde{\varepsilon}_{12} & \tilde{\varepsilon}_{13} \\ \tilde{\varepsilon}_{21} & \tilde{\varepsilon}_{22} & \tilde{\varepsilon}_{23} \\ \tilde{\varepsilon}_{31} & \tilde{\varepsilon}_{32} & \varepsilon_{33} \end{bmatrix} \begin{bmatrix} \tilde{\varepsilon}_{11} & \tilde{\varepsilon}_{12} & \tilde{\varepsilon}_{13} \\ \tilde{\varepsilon}_{21} & \tilde{\varepsilon}_{22} & \tilde{\varepsilon}_{23} \\ \tilde{\varepsilon}_{31} & \tilde{\varepsilon}_{32} & \varepsilon_{33} \end{bmatrix} \tag{290}$$

To derive the expression for the second order variation of B due to two different virtual crack extensions, δa_i and δa_j, one can use the relationship

$$\frac{\delta \varepsilon_i}{\delta a_j} = \varepsilon_{i,j} = -\varepsilon_j \varepsilon_i \tag{291}$$

which yields an expression similar to equation 289 for $\dfrac{\delta^2 B}{\delta a_i \delta a_j}$

$$\frac{\delta^2 B}{\delta a_i \delta a_j} = -\begin{bmatrix} \lfloor \tilde{\underline{\varepsilon}}_1" \rfloor & & \\ & \lfloor \tilde{\underline{\varepsilon}}_2" \rfloor & \\ & & \lfloor \tilde{\underline{\varepsilon}}_3" \rfloor \\ \lfloor \tilde{\underline{\varepsilon}}_2" \rfloor & \lfloor \tilde{\underline{\varepsilon}}_1" \rfloor & \\ & \lfloor \tilde{\underline{\varepsilon}}_3" \rfloor & \lfloor \tilde{\underline{\varepsilon}}_2" \rfloor \\ \lfloor \tilde{\underline{\varepsilon}}_3" \rfloor & & \lfloor \tilde{\underline{\varepsilon}}_1" \rfloor \end{bmatrix} \begin{bmatrix} \frac{\partial N}{\partial x^1} & & \\ \frac{\partial N}{\partial x^2} & & \\ \frac{\partial N}{\partial x^3} & & \\ & \frac{\partial N}{\partial x^1} & \\ & \frac{\partial N}{\partial x^2} & \\ & \frac{\partial N}{\partial x^3} & \\ & & \frac{\partial N}{\partial x^1} \\ & & \frac{\partial N}{\partial x^2} \\ & & \frac{\partial N}{\partial x^3} \end{bmatrix} \tag{292}$$

in which $\lfloor \tilde{\underline{\varepsilon}}_1" \rfloor$, $\lfloor \tilde{\underline{\varepsilon}}_2" \rfloor$ and $\lfloor \tilde{\underline{\varepsilon}}_3" \rfloor$ are the component matrices of $\left[\tilde{\underline{\varepsilon}}" \right]$ defined by

$$\tilde{\underline{\varepsilon}}" = \begin{Bmatrix} \lfloor \tilde{\underline{\varepsilon}}_1" \rfloor \\ \lfloor \tilde{\underline{\varepsilon}}_2" \rfloor \\ \lfloor \tilde{\underline{\varepsilon}}_3" \rfloor \end{Bmatrix} = \left[\varepsilon_j \right] \left[\varepsilon_i \right] + \left[\varepsilon_i \right] \left[\varepsilon_j \right] \tag{293}$$

The first and second order variations of $|J|$ with respect to virtual crack extension, δa_i, at a point i on crack front are defined as

$$\frac{\delta|J|}{\delta a_i} = Tr(\tilde{\varepsilon})|J| \tag{294}$$

$$\frac{\delta^2|J|}{\delta a_i^2} = \left(Tr^2(\tilde{\varepsilon}) - Tr(\tilde{\varepsilon}^2)\right)|J| \tag{295}$$

The second order variation of $|J|$ with respect to two different virtual crack extensions, δa_i and δa_j, is written as

$$\frac{\delta^2|J|}{\delta a_i \delta a_j} = \left(Tr(\tilde{\varepsilon}_i)Tr(\tilde{\varepsilon}_j) - Tr(\tilde{\varepsilon}_j\tilde{\varepsilon}_i)\right)|J| \tag{296}$$

The first and second order variations of element stiffness matrix are written as

$$\frac{\delta k}{\delta a_i} = \int_v \left[\frac{\delta B}{\delta a_i}^T DB + B^T D\frac{\delta B}{\delta a_i} + Tr(\tilde{\varepsilon})B^T DB\right] dV \tag{297}$$

$$\begin{aligned}\frac{\delta^2 k}{\delta a_i^2} = \int_v \Bigg[&\frac{\delta^2 B}{\delta a_i^2}^T DB + 2\frac{\delta B}{\delta a_i}^T D\frac{\delta B}{\delta a_i} + B^T D\frac{\delta^2 B}{\delta a_i^2} + \left(Tr^2(\tilde{\varepsilon}) - Tr(\tilde{\varepsilon}^2)\right)B^T DB \\ &+ 2Tr(\tilde{\varepsilon})\left(\frac{\delta B}{\delta a_i}^T DB + B^T D\frac{\delta B}{\delta a_i}\right)\Bigg] dV\end{aligned} \tag{298}$$

The second order variation of element stiffness, $\frac{\delta^2 k}{\delta a_i \delta a_j}$, with respect to two different virtual crack extensions, δa_i and δa_j, is written as

$$\frac{\delta^2 k}{\delta a_i \delta a_j} = \int_v \left[\frac{\delta^2 B}{\delta a_i \delta a_j}^T DB + \frac{\delta B}{\delta a_i}^T D\frac{\delta B}{\delta a_j} + \frac{\delta B}{\delta a_j}^T D\frac{\delta B}{\delta a_i} + B^T D\frac{\delta^2 B}{\delta a_i \delta a_j}\right.$$

$$+\left(Tr\left(\tilde{\varepsilon}_i\right)Tr\left(\tilde{\varepsilon}_j\right)-Tr\left(\tilde{\varepsilon}_j\tilde{\varepsilon}_i\right)\right)B^T DB+Tr\left(\tilde{\varepsilon}_i\right)\left(\frac{\delta B}{\delta a_j}^T DB+B^T D\frac{\delta B}{\delta a_j}\right)$$

$$+Tr\left(\tilde{\varepsilon}_j\right)\left(\frac{\delta B}{\delta a_i}^T DB+B^T D\frac{\delta B}{\delta a_i}\right)\Bigg]dV \qquad (299)$$

In the case of a system of 2D multiple cracks, Section 5, the elements influenced by each crack-tip comprised disjoint sets and thus the second order variations of stiffness and loading with respect to two different crack extensions a_i and a_j vanished. On the contrary, in the 3D case, the second order stiffness derivatives due to two different crack extensions on the crack front are not necessarily zero, because areas perturbed due to different crack extensions along the crack front may be overlapped, Figure 70, and then the interaction between crack front perturbations should be taken into account. For the linear virtual crack extension along the crack front, the elements influenced by virtual crack extension at one point are also affected by the extensions at adjacent points. The shadowed portion in Figure 70 represents the crack front perturbation area simultaneously affected by virtual crack extensions at two neighboring positions. Therefore, for the linear virtual crack front perturbation in Figure 67a, the second order variations of element stiffness are

$$\frac{\delta^2 k}{\delta a_i \delta a_j}\neq 0, \quad \frac{\delta^2 f}{\delta a_i \delta a_j}\neq 0 \quad \text{for } j=i-1,\ i \text{ or } i+1 \qquad (300)$$

$$\frac{\delta^2 k}{\delta a_i \delta a_j}=0, \quad \frac{\delta^2 f}{\delta a_i \delta a_j}=0 \quad \text{otherwise} \qquad (301)$$

Element stiffness variations, $\delta k/\delta a_i$, $\delta^2 k/\delta a_i^2$ and $\delta^2 k/\delta a_i \delta a_j$ are assembled to produce the global stiffness variations $\delta K/\delta a_i$, $\delta^2 K/\delta a_i^2$ and $\delta^2 K/\delta a_i \delta a_j$, respectively.

6.1.4 Crack-face, thermal and body force loadings in three dimensions

The elemental equivalent load variations associated with crack extension for a non-uniform crack-face pressure, *p*, are given by,

$$f_e = \int_s N^T p \ \ ds \tag{302}$$

$$\frac{\delta f_e}{\delta a_i} = \int_s \left[N^T \frac{\delta p}{\delta a_i} + Tr(\tilde{\varepsilon}) N^T p \right] ds \tag{303}$$

$$\frac{\delta^2 f_e}{\delta a_i^2} = \int_s \left[N^T \frac{\delta^2 p}{\delta a_i^2} + 2Tr(\tilde{\varepsilon}) N^T \frac{\delta p}{\delta a_i} + \left(Tr^2(\tilde{\varepsilon}) - Tr(\tilde{\varepsilon}^2) \right) N^T p \right] ds \tag{304}$$

$$\frac{\delta^2 f_e}{\delta a_i \delta a_j} = \int_s \left[N^T \frac{\delta^2 p}{\delta a_i \delta a_j} + Tr(\tilde{\varepsilon}_i) N^T \frac{\delta p}{\delta a_j} + Tr(\tilde{\varepsilon}_j) N^T \frac{\delta p}{\delta a_i} \right.$$

$$\left. + \left(Tr\left(\tilde{\varepsilon}_i\right) Tr\left(\tilde{\varepsilon}_j\right) - Tr\left(\tilde{\varepsilon}_j \tilde{\varepsilon}_i\right) \right) N^T p \right] ds \tag{305}$$

where N is the shape function matrix and *ds* is an unit crack-face area.

In the same manner, the variations of thermal loading for an isotropic material can be derived as,

$$f_e = \int_v B^T D(\alpha \Delta T) \ dV \tag{306}$$

$$\frac{\delta f_e}{\delta a_i} = \int_v \left[\frac{\delta B}{\delta a_i}^T D(\alpha \Delta T) + B^T D \frac{\delta(\alpha \Delta T)}{\delta a_i} + Tr(\tilde{\varepsilon}) B^T D(\alpha \Delta T) \right] dV \tag{307}$$

$$\frac{\delta^2 f_e}{\delta a_i} = \int_v \left[\frac{\delta^2 B}{\delta a_i^{\ 2}}^T D(\alpha\Delta T) + 2\frac{\delta B}{\delta a_i}^T D\frac{\delta(\alpha\Delta T)}{\delta a_i} + B^T D\frac{\delta^2(\alpha\Delta T)}{\delta a_i^{\ 2}} \right.$$
$$\left. + 2Tr(\tilde{\varepsilon})\left(\frac{\delta B}{\delta a_i}^T D\alpha\Delta T + B^T D\frac{\delta(\alpha\Delta T)}{\delta a_i}\right) + \left(Tr^2(\tilde{\varepsilon}) - Tr(\tilde{\varepsilon}^2)\right)B^T D\frac{\delta(\alpha\Delta T)}{\delta a_i}\right] dV$$

(308)

$$\frac{\delta^2 f_e}{\delta a_i \delta a_j} = \int_v \left[\frac{\delta^2 B}{\delta a_i \delta a_j}^T D(\alpha\Delta T) + \frac{\delta B}{\delta a_i}^T D\frac{\delta(\alpha\Delta T)}{\delta a_j} + \frac{\delta B}{\delta a_j}^T D\frac{\delta(\alpha\Delta T)}{\delta a_i} + B^T D\frac{\delta^2(\alpha\Delta T)}{\delta a_i \delta a_j} \right.$$
$$+ \left(Tr(\tilde{\varepsilon}_i)Tr(\tilde{\varepsilon}_j) - Tr(\tilde{\varepsilon}_j\tilde{\varepsilon}_i)\right)B^T D(\alpha\Delta T) + Tr(\tilde{\varepsilon}_i)\left(\frac{\delta B}{\delta a_j}^T D(\alpha\Delta T) + B^T D\frac{\delta(\alpha\Delta T)}{\delta a_j}\right)$$
$$\left. + Tr(\tilde{\varepsilon}_j)\left(\frac{\delta B}{\delta a_i}^T D(\alpha\Delta T) + B^T D\frac{\delta(\alpha\Delta T)}{\delta a_i}\right)\right] dV \qquad (309)$$

6.1.5 Mixed-mode fracture problem

The crack-tip field parameters (displacements, stresses, strains and tractions) within the symmetric region in the crack tip neighborhood along the straight crack front can be separated into mode *I*, *II* and *III* components. Nodal displacement vector and load vector, u and f are decomposed into mode *I*, *II*, and *III* as,

$$\{u\} = \{u^I\} + \{u^{II}\} + \{u^{III}\} = \frac{1}{2}\begin{Bmatrix} u_1 + u_1' \\ u_2 - u_2' \\ u_3 + u_3' \end{Bmatrix} + \frac{1}{2}\begin{Bmatrix} u_1 - u_1' \\ u_2 + u_2' \\ 0 \end{Bmatrix} + \frac{1}{2}\begin{Bmatrix} 0 \\ 0 \\ u_3 - u_3' \end{Bmatrix}$$

(310)

$$\{f\} = \{f^I\} + \{f^{II}\} + \{f^{III}\} = \frac{1}{2}\begin{Bmatrix} f_1 + f_1' \\ f_2 - f_2' \\ f_3 + f_3' \end{Bmatrix} + \frac{1}{2}\begin{Bmatrix} f_1 - f_1' \\ f_2 + f_2' \\ 0 \end{Bmatrix} + \frac{1}{2}\begin{Bmatrix} 0 \\ 0 \\ f_3 - f_3' \end{Bmatrix}$$

(311)

where $$u_i'(x_1, x_2, x_3) = u_i(x_1, -x_2, x_3) \quad (312)$$

$$f_i'(x_1, x_2, x_3) = f_i(x_1, -x_2, x_3) \quad (313)$$

The total energy release rate, under mixed-mode loading at any point along a three-dimensional crack front for unit crack extension, is given by

$$G_i = (G_I)_i + (G_{II})_i + (G_{III})_i \quad (314)$$

By decomposing the computed displacement and loading fields into mode *I, II* and *III* components, one may evaluate energy release rate components G_I, G_{II} and G_{III}, as

$$(G_I)_i = -\frac{1}{2}(u_I)^T \frac{\delta K}{\delta a_i} u_I + (u_I)^T \frac{\delta f_I}{\delta a_i} \quad (315)$$

$$(G_{II})_i = -\frac{1}{2}(u_{II})^T \frac{\delta K}{\delta a_i} u_{II} + (u_{II})^T \frac{\delta f_{II}}{\delta a_i} \quad (316)$$

$$(G_{III})_i = -\frac{1}{2}(u_{III})^T \frac{\delta K}{\delta a_i} u_{III} + (u_{III})^T \frac{\delta f_{III}}{\delta a_i} \quad (317)$$

For an arbitrarily-shaped crack front, it is not straightfoward to use the mode decomposition technique. In this case, a point-by-point co-ordinate transformation from a global Cartesian co-ordinate system to the local crack front co-ordinate system can be performed prior to the calculation of energy release rate and its derivatives (Nikishkov, 1987). After the transformation, the crack front is straight and the mode decomposition technique can be applied.

6.2 *Numerical Examples*

In this section, a series of numerical examples are presented and compared with results existing in the literature to demonstrate the accuracy of the proposed method.

6.2.1 *Example 5: Embedded penny-shaped crack in a large cylinder under a remote uniform tensile loading normal to the crack plane*

The first example is a penny-shaped crack of radius a=1.0 in a large cylindrical body subjected to a remote tensile load perpendicular to the crack surface. A large cylinder with *R/a*=20 and *H/a*=20 simulates the infinite domain, Figure 71a. Figure 71b shows nodes defined on the crack front. Due to the symmetry in the problem, only 1/8 of the cracked cylinder was considered. The mesh used for the penny-shaped crack is shown in Figure 71c. The finite element mesh consists of 432 elements and 3263 nodes. The detail of the mesh around the crack front is shown in Figure 71d. The quarter-point 15-noded wedge elements were employed to model the singularity around the crack front. Young's modulus *E* was taken to be unity, and Poisson's ratio 0.3. The exact K_I and $\delta K_I / \delta a$ solutions for Mode-I crack growth under uniform stress in an infinite domain can be expressed analytically (Sneddon, 1946) as,

$$K_I = 2\sigma\sqrt{\frac{a}{\pi}} \tag{318}$$

$$\frac{\delta K_I}{\delta a} = \frac{\sigma}{\sqrt{a\pi}} \tag{319}$$

It is noted that the virtual crack extension is given in the direction normal to the crack front such that it produces self-similar crack growth. For *R/a* = 20, the present virtual crack extension method gives K_I =1.1302 for all θ which is in excellent agreement with the exact solution of 1.1284 by equation (318), giving error of 0.16 % for this mesh.

Table 14 lists the values of rates of stress intensity factor computed with the present virtual crack extension method. The sums of the rows in Table 14 represents the rate of stress intensity factor at all nodes along the crack front, due to an uniform extension of a entire crack front. The theoretical value of $\delta K_I / \delta a$ by equation (319) for axisymmetric case is 0.5642 for all θ. The difference between the computed and theoretical $\delta K_I / \delta a$ values is about 4 %.

To demonstrate the accuracy of the present method, the stress intensity factors $K_i^{Ellipse}$ for several elliptical cracks are approximated, based on the known values of the stress intensity factors K_i^{Circle} and their rates $\partial K_i^{Circle} / \partial a_j$ for the current penny-shaped crack front, and using the linear relation, Figure 72:

$$K_i^{Ellipse} = K_i^{Circle} + \frac{\partial K_i^{Circle}}{\partial a_j} \delta a_j \qquad (320)$$

Comparison of the extrapolated stress intensity factors with a reference solution (Irwin, 1962) is given in Table 15. Close agreement with the reference solution was obtained.

6.2.2 Example 6: Semi-circular surface crack in a half- cylinder under a remote uniform tensile loading normal to the crack plane

A half-cylinder containing a semi-circular surface crack subjected to a remote uniform tensile loading normal to the crack plane is shown in Figure 73. The mesh used is the same as that for the penny-shaped crack in Example 5 and the only change occurs in the boundary conditions of the two vertical surfaces intercepting the crack surface that were previously supported by rollers. The flat face becomes free for the half-cylinder problem. Table 16 shows the comparison of the stress intensity factor calculated by the present method with the reference solution by Newman and Raju (1981), where the stress intensity factor was normalized by $K_0 = 2\sigma\sqrt{a/\pi}$ for a penny-shaped embedded crack. As illustrated in Figure 74, good agreement was obtained at all locations along the crack front.

Table 17 lists the calculated stress intensity factor derivatives for a semi-circular surface crack. Since there have been no published values for derivatives of the stress intensity factor, verification with other reference solutions is not straightforward. One way to evaluate the accuracy of the proposed method for $\delta K_I / \delta a$ is to compare extrapolated results seems to judge from the stress intensity factors extrapolated to semi-elliptical surface cracks, based on the known values of the stress intensity factors and their rates on the current semi-circular crack front, Figure 75. In Table 18, the results for b/a=1.2 and 1.4 are presented. In all cases, the maximum difference between the extrapolated value and the reference solution is less than 3%.

6.2.3 *Example 7: A center-cracked plate subjected to a remote uniform tensile loading normal to the crack plane*

The next numerical example investigates a center-cracked plate subjected to a remote uniform tensile loading, $\sigma = 1.0$, perpendicular to the crack surface, Figure 76a. The present analysis is carried out on specimens of the following dimensions: (a) *W=H*=20.0, *t*=4.0, *a=1.0* (b) *W=H*=20.0, *t*=4.0, *a=8.0*. Using the symmetry in the problem, only 1/8 of the plate was considered. The finite element mesh consists of 432 elements and 3263 nodes for case (a), Figure 76b, and 516 elements and 3681 nodes for case (b). The quarter-point 15-noded wedge elements were employed to model the singularity around the crack front, Figure 76d. The crack tip element size was taken to be 1/8 of crack length *a*. It is noted that the result for $\nu = 0.0$ is identical to the 2D solution with the same Poisson's ratio and thus comparison of the results with reference solutions is possible. For *W/a*=20.0 and $\nu = 0.0$, the present analysis gave *G*=3.1757 and $\delta G / \delta a$ =3.1518 which are in excellent agreement with the reference values for a 2D crack (Ishida, 1971), Tables 19 and 21. For *W/a*=2.5, *W* being the same as before, the value computed for *G* by the present method is 37.367 which again is in correspondence with the value of 37.167 obtained using solutions of Ishida, Table 20.

The distribution of energy release rates along the crack front is shown in Figure 77 for different Poisson's ratios and the following geometries (a) *W=H*=20.0, *t*=4.0, *a=1.0* (b) *W=H*=20.0, *t*=4.0, *a=8.0*. The local energy release rate around the crack front is normalized by K_I^2 / E in which K_I is the reference stress intensity factor for a 2D crack. Figure 77 shows that, as one approaches the free surface, the energy release rate value decreases. This boundary layer effect was observed by Hartranft and Sih (1970). The thickness of this layer is given by,

$$\frac{\varepsilon}{t} = \frac{1}{4 + 16t/a} \qquad (321)$$

This is an approximate measure of the region within which the surface effects are significant (Narayana, 1994). The boundary layer thickness ε / t is 0.0147 and 0.08333 for the cases (a) *t/a=4.0* and (b) *t/a=0.5*, respectively. In order to show this reduction for the case (a) *t/a=4.0*, a much finer mesh near the free surface would be required. In the case of *t/a=0.5*, the boundary layer effect is clearly illustrated in Figure 77b.

6.3 Summary

In this Section, the analytical virtual crack extension method introduced by Lin and Abel (1988) is generalized to a three-dimensional crack problem. The general derivations are given for energy release rates and their higher derivatives of a three-dimensional planar crack of arbitrary shape under arbitrary loading conditions. The present method maintains all the advantages of the similar virtual crack extension techniques (deLorenzi 1982, 1985; Haber, 1985; Barbero, 1990) and adds the capability of calculating higher order derivatives of energy release rate for a three-dimensional crack of arbitrary shape. The method provides the direct integral forms of stiffness derivatives for 3D finite elements, and thus there is no need for the analyst to specify a finite length of virtual crack extension. The salient feature of this method is that the energy release rates and their higher derivatives for three-dimensional cracks of arbitrary shape can be computed in a single analysis. Furthermore, this generalized formulation for the 3D crack problem has a couple of new features. First, the present method considers the interaction between virtual crack extensions at different positions along the crack front, because the areas perturbed due to crack extensions at adjacent positions on the front are overlapped. The additional term representing the interaction between virtual crack extensions is explicitly derived and included in the formulation for the second variations of element stiffness. Secondly, it is shown that a local curvature on the curved crack front must be taken into account to properly calculate the derivatives of energy release rate. The general formula for the derivatives of energy release rates around an arbitrarily curved front is provided.

Several 3-D numerical examples with exact solutions or with solutions available in the literature are solved to demonstrate the accuracy of the current method. It was shown that the maximum computed errors were about 0.2 % for energy release rate, and 2-4 % for its first derivative between the simulated solutions and the reference solutions for the mesh density used in the examples. Accuracy can be improved with mesh refinement according to the guidelines provided herein. The proposed method has immediate application to the following related problems: the shape prediction and stability analysis of an evolving 3D crack front in fatigue or brittle fracture; configurational stability in fatigue crack propagation prediction; investigation of bifurcation in brittle fracture.

The variational methodology described in Sections 5 and 6 can be applied to even further generalizations of the LEFM crack growth problem. These include:

- Non-colinear growth of 2D cracks. Section 4 presented various techniques for predicting the trajectory and stability of a 2D crack. One could take an alternative approach based on the principle of minimum potential energy to discover the trajectory of a non-colinear 2D crack or trajectories of a system of interacting non-colinear cracks. The methods described in Section 5 would be used to calculate the energy release rates and their derivatives necessary for such an approach. Some work on this problem is reported in Hwang (1999) and Hwang and Ingraffea (2002).
- Non-coplanar growth of a 3D crack. Again, one could take an approach based on the principle of minimum potential energy to discover the shape of such a crack. The methods described in Section 6 would be used to calculate the energy release rates and their derivatives necessary for this problem.