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Finite Element Analysis of a Semi-elliptical Crack Embedded at the Notch Root in a Single Crystal Bar

by

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fulfillment of the requirements for the degree of

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Abstract

In this research, a single-notch bar of single crystal superalloy PWA 1480 was studied with the finite element method (FEM). Stress and strain concentrations at the notch under different levels of tensile loading were investigated, considering two typical notch orientations in terms of material [110] and [100] directions, based on anisotropic material properties. Orientation dependence of the notch effect on the stress and strain concentrations was discussed. The FEM model of the single notch bar was further complicated with embedding a semi-elliptical crack at the notch root. The pointwise J integral along the semi-elliptical crack front and the crack opening displacement (COD) behind two typical crack front positions, which are in the short and long semi-axes respectively, were evaluated respectively for the two notch orientations at different tensile load levels. Three crack sizes were considered in the model in order to investigate the crack size effect on the crack tip characteristic parameters, such as J integral, COD and crack tip opening displacement (CTOD). The anisotropic effect on the J integral was also compared with that of isotropic materials. A correlation was established between the J integrals of a semi-elliptical crack front point and a through-the-thickness crack evaluated based on the continuously distributed dislocation theory (CDDT). Finally, the correlation factor n between the J integral and CTOD was evaluated, similarly to isotropic material, based on the elastic-plastic fracture mechanics (EPFM).

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Nomenclature

a	Crack length, or short semi-axis of semi-elliptical crack
A	Correlation parameter in elastic-plastic stress-strain equation
$\bar{a}$	Equivalent crack length
ASTM	American Society for Testing and Materials
c	Long semi-axis of semi-elliptical crack
C	Material constant in Paris and Erdogan equation
$\mathbf{C}$	Stiffness matrix
CDDT	Continuously distributed dislocation theory
COD	Crack opening displacement
CTOD	Crack tip opening displacement
d	Half single notch bar thickness
da/dN	Fatigue crack propagation rate
E	Young's modulus
EPFM	Elastic-plastic fracture mechanics
FCC	Face-centered cubic
FEM	Finite element method
F, G, H, L, M, N	Material constants defined in Hill's potential function
F_{sn}	Boundary correction factor of stress intensity factor
g	Hardening factor in elastic-plastic stress-strain equation
G	Potential energy release rate
$\bar{G}$	Equivalent potential energy release rate
$[h\ k\ l]$	Miller indices of direction
I_g	Correlation parameter in elastic – plastic stress and strain equations
J	J integral
J_{IC}	EPFM fracture toughness
k	Parameter in equation of stress intensity factor of semi-elliptical crack

K	Stress intensity factor
K_I	Mode I stress intensity factor
K_{IC}	Fracture toughness for mode I loading condition
K_t	Stress concentration factor
K_ϵ	Strain concentration factor
LEFM	Linear elastic fracture mechanics
m	Parameter in Paris and Erdogan equation
n	Parameter in J and CTOD relation equation
$\mathbf{n}$	Direction vector normal to crack plane
NASA	National Aeronautics and Space Administration
NRC	National Research Council of Canada
$J_{\Gamma_1}, J_{\Gamma_2}$	J integral along different integral path
q	Coefficient of energy release rate
$\mathbf{q}$	Direction vector in crack extension
Q	Coefficient of stress intensity factor
$[Q]$	Relationship matrix in coordinate transformation
r	Distance from crack tip
R	Stress ratio of cyclic loading
R_{ij}	Anisotropic yield stress ratio
r_p	Crack tip plastic zone radius
$\mathbf{S}$	Compliance matrix
SC	Single crystal
SCF	Strain concentration factor
SIF	Stress intensity factor
$\mathbf{t}$	Direction vector tangent to crack front
$t_2^F, t_2^0, F_{22}^{-1}$	Parameters in Wu's equation of energy release rate
V	Potential energy of cracked solid
W	Strain energy density
α, β, γ	Direction cosines of two coordinate system
θ	Polar angle in a cylindrical coordinate system

ΔJ	J integral range corresponding to the loading frame
ΔK	Stress intensity factor range
ΔK_{th}	Threshold stress intensity factor range
$\Delta \sigma$	Stress range of a cyclic loading
γ_{ij}	Shearing strain components
ε_{max}	Maximum strain at the stress concentration point
ε_{nom}	Nominal strain
ε_{pe}	Equivalent plastic strain
σ_{ij}	Stress components
$\bar{\sigma}_{ij}$	Yielding stress in a certain direction of an anisotropic material
σ_{max}	Maximum stress at stress concentration area or in cyclic loading
σ_{min}	Minimum stress in cyclic loading
σ_{nom}	Nominal stress
σ^o	Reference yielding strength
σ_e	Equivalent stress
σ_s	Yielding strength
σ_x	Tensile stress in x direction
σ_{ymax}	Maximum stress in tension direction
ν	Poisson's ratio
τ^o	Reference shear strength
Γ	Integration loop around the crack tip
ϕ	Elliptical angle
λ	CTOD coefficient

Chapter 1

Introduction

1.1 Objectives

This research is aimed to:

- (1) evaluate the strain concentration factor of a notched bar under elastic-plastic deformation, emphasizing the effect of material orientation on strain concentration, taking PWA 1480 SC superalloy as an example;
- (2) evaluate the elastic-plastic crack tip stress-strain field parameters, J integral, crack opening displacement (COD) and crack tip opening displacement (CTOD) at the front of a semi-elliptical crack embedded at the notch root of a PWA 1480 single crystal (SC) bar under elastic- plastic loading condition;
and
- (3) study the effects of crack tip position, crack size, loading level and material orientation on the above parameters of the crack tip stress-strain fields.

1.2 Research Background

Gas turbine engines are widely used in modern aviation industry and electric power plants. They may also be used for powering boats, trains, automobiles and trucks. Gas turbine engine components such as turbine disks, blades and guide vanes, which operate in the most arduous conditions of temperature and stress of any component in the engine, are often pushed to their endurance limit in order to increase weight savings and thrust. The service condition of the turbine section usually induces hot corrosion, fatigue and creep due to high stress and temperature, as well as thermal fatigue due to temperature transients [1]. All of these conditions contribute to crack initiation and propagation in turbine components. The propagation of cracks in these components greatly affects their fatigue life and may directly cause their failure. For example, turbine discs and turbine blades in aircraft engines are safety-critical components where the propagation of a crack may lead to failure of the components, thus resulting in catastrophic loss of the engine and possibly the whole airplane. Failure of an individual turbine blade may also cause so-called secondary damage to other blades at the same blade stage and in the downstream. Therefore, cost savings and safety benefits in successfully predicting time to failure in both types of components are evident, allowing for appropriate safety checks and maintenance schedules.

The elaborated air cooling configuration of modern turbine airfoils greatly improves their temperature endurance by bleeding pressurized air from engine compressor through the internal passages of these components, but this introduces more

stress concentration features to the geometry. The stress concentration can become more serious in the turbine blade firtree region (Figure 1.1) below the platform where a variety of notch geometries are usually present [1]. Cracks in this region may be initiated by local high stress level and elevated temperature, which is relatively lower compared with the temperature of the upper part of the blade. Since modern turbine airfoils are usually made of single crystal superalloys, which possess distinctive material anisotropy, the crack propagation behaviour in the turbine airfoil can be affected by the material's anisotropic properties, which needs to be addressed using either linear elastic fracture mechanics (LEFM) or elastic-plastic fracture mechanics (EPFM) for anisotropic bodies.

The propagation of long fatigue cracks in polycrystalline materials can be well evaluated in terms of LEFM, in which the small yielding effect at crack tip is overcome by elastic assumptions [2], and the cracked solid material is assumed isotropic. Within the LEFM range, the stress intensity factor (SIF) K is a sufficient parameter to describe the whole stress field at the tip of a crack. Also a well developed empirical relationship in fatigue life prediction, Paris and Erdogan equation [3], shows that the fatigue crack propagation rate per cycle, da/dN , is governed by the stress intensity factor range, ΔK :

$$da/dN = C(\Delta K)^m, \quad (1.1)$$

where C and m are constants that may be determined experimentally.

However, LEFM is invalid to describe the propagation behaviour of a short crack, which usually consumes large percentage of the fatigue lifetime of a turbine component. Before any discussion of short crack behaviour, a question must be answered firstly, in

what size may a crack be considered as short crack? A general idea of short crack was shown schematically in Kitagawa-Takahashi diagram [4] (Figure 1.2), in which the short crack was sub-divided into two regimes, microstructurally short crack and physically short crack. The first short crack regime was limited within one grain size, while the second regime may be defined in several methods as suggested by Taylor [4,5]. A crack was considered short if either its size was within ten grains in polycrystalline materials, or less than $1000 \mu\text{m}$, or within the same order as the crack tip plastic zone when the latter was compared with crack length itself. Since Pearson [6] emphasized that short fatigue crack could propagate much faster than long fatigue cracks under the same ΔK , considerable research has been made to investigate the anomalous behaviour of short fatigue cracks [4-17]. Although the short crack anomaly was not observed in some experimental work on turbine component alloys [18-20], most experimental evidence has shown that as a crack-growth-rate correlation parameter, the LEFM cyclic stress intensity factor range ΔK in equation (1.1) failed to consistently describe the short fatigue crack growth process especially when it happened below the so-called fatigue crack growth threshold for long cracks, ΔK_{th} . Reed *et al.* [16] reported a remarkable crystal orientation dependence of Paris relationship in investigating the fatigue crack behaviour of a nickel-based SC. Also, ample research [4,9,10, 13-17] showed that the characteristic material constant C in equation (1.1) failed to uniquely characterize anisotropic material properties. It has been realized that anomalous behaviour of both the short cracks or cracks in single crystal is closely attributed to the intrinsic microstructure properties of materials, grain boundary blocking effects [10, 13,14] and material anisotropy [12], which are generally omitted for cracks in a polycrystalline solid. However current

formulations of LEFM and EPFM methods rely mostly on the use of isotropic fracture mechanics parameters and models, which do not consider material microstructure and crystallographic features [9,15]. To find a fundamentally sound and physically consistent description for short cracks or cracks in single crystals, this issue needs to be addressed with consideration of crystalline anisotropy. Since SC materials, such as those used in engine turbine section, can be considered both as engineering materials with complex anisotropic failure issues that need to be evaluated and as a model for the early stages of short crack growth in polycrystalline materials, where local crystal anisotropy issues also hold great importance, a series of work including metallurgical study, fatigue testing, and theoretical modeling of cracks in SC superalloys have been under way.

The group of X. P. Zhang, C. H. Wang, L. Ye and Y. W. Mai [7, 8, 11] from University of Sydney, Australia has conducted a research on in-situ SEM investigation of short fatigue cracks in poly-crystal and SC alloys. The short crack fatigue tests were carried out on aluminum alloys and nickel-base superalloys. The experimental results reveal that fatigue cracks may grow in a shear decohesion mode over a length several times the grain size, far beyond the conventional stage I regime. For the nickel-base SC superalloy, it was observed that there did exist the so-called anomaly of short fatigue crack growth, similar to polycrystalline alloys; and that mode I fatigue cracks grew along the shear band with the loading axis being nearly perpendicular to the main shear plane of the single crystal. Compared to poly-crystals, fatigue crack growth in single crystal alloy exhibited less deflected crack path and fairly flat fracture surfaces. These imply the effect of material microstructure orientations on the path of short crack propagation.

The group of P.A.S. Reed, J.E. King, X.D. Wu and I. Sinclair [16, 21, 22] from University of Southampton, United Kingdom has investigated the effect of material orientation, applied stress state, environment, and temperature on the crack growth and crack-path behaviour of SC nickel-base alloy. Consideration of the local resolved shear-stress intensity and local resolved normal-stress intensity for each slip system allows the prediction of stage I crack paths, clarifying the importance of secondary single crystal testing orientation. A combination of both opening and shearing was found to promote stage I crack growth, and boundary conditions were established within which stage I cracking is promoted. Highly deflected stage I cracking gave rise to significant shielding effects, but under suitable mixed-mode loading, highly oriented, coplanar stage I crack growth could be produced. A remarkable crystal orientation dependence of Paris relationship was reported in their research.

The group of X. J. Wu, A.K. Koul, A.S. Krausz and J. P. Immarigeon (12, 23, 24) from National Research Council of Canada (NRC) have been carrying out a series of research on fatigue crack growth in SC superalloys. Wu. *et al.* have proposed an elastic-plastic fracture model for mixed mode I-II and mode III cracks in anisotropic materials with perfect plastic behaviour, based on the continuously distributed dislocation theory (CDDT), and demonstrated the application of the model to long fatigue cracks in nickel-base SC superalloy and small crack within a grain. In this model, the distribution of elastic-plastic strain in the yielded region is represented by an inverted pile-up of dislocations, and the CTOD and energy release rate, G , of a yielded crack, are obtained in close forms. For SC superalloys under small-scale yielding conditions, it appears that

both CTOD and G are appropriate parameters for consolidating fatigue-crack-growth rate data, whereas the correlation with ΔK is orientation dependent.

The above research activities emphasize the effect of material anisotropy on the mechanism of either short crack propagation in microstructural region or long crack propagation in SC superalloys. They provide a solid background to a current collaborative research on short cracks in anisotropic materials, involving collaboration between the Structures, Materials and Propulsion Laboratory of the Institute for Aerospace Research, National Research Council of Canada, the Materials Group of the School of Engineering Sciences, at Southampton University, UK and Carleton University. This joint project may lead to a unified elastic-plastic fracture mechanics model for description of fatigue crack growth in both polycrystalline and SC materials, supported by experimental and numerical results, particularly in the presence of complex stress states, such as those found at a stress concentrator feature.

1.3 Current work

This thesis forms a part of the ongoing joint project in simulating a single-notch bar with finite element method (FEM). The purpose of the present work is to investigate the influence of material orientation on the strain concentration of a through-the-thickness SC single-notch bar under elastic-plastic uniaxial tensile loading, and the characteristic parameters of the stress-strain field along the front of a semi-elliptical crack embedded at notch root of the single-notch bar. Based on the numerical results of different notch orientations, crack sizes, and loading levels, the material anisotropy

effects on strain concentration factor, J integral distribution, COD, and CTOD are discussed. The finite element models were created to simulate the fracture behaviour of the turbine components, where cracks usually originate from the local stress concentrations caused by the unavoidable stress raisers, for example, fillets, grooves, or notches. The numerical results can be useful in the fatigue crack life prediction of gas turbine engine components, such as SC turbine airfoil.

A stress or strain concentration analysis of notches always holds great importance to understand the crack initiation condition because the actual behaviour of cracks may be greatly influenced by local plastic-strain fields at local geometry discontinuities [25-27]. In fracture analysis, a notch together with semi-elliptical surface crack or quarter-elliptical cracks is often considered because they are the best representations of natural cracks, which are usually found initiated from surface stress raiser or at edges. Detailed analysis of stress concentration at a notch has been published for both elastic and fully plastic body [28, 29], while semi-elliptical surface crack has also received much attention in literature [30-35]. However, the material anisotropy was seldom involved in the previous work. Review of the earlier studies on semi-elliptical crack found that numerical methods had been widely used in evaluating the crack tip field characteristic parameter, stress intensity factor (SIF), J integral or CTOD, especially in EPFM [36-45]. Due to the complex stress and strain distribution and the absence of analytical solution for anisotropic fracture problems, FEM was reasonably employed in solving this problem. Numerical model of a single-notch bar of SC superalloy PWA 1480 was conducted using the commercial FEM package ABAQUS, which has been widely used in research and

reported satisfactory correlation with either analytical or experiment methods [37-39, 44,45].

1.4 Organization of the Thesis

This thesis consists of five chapters. Section 1.1, 1.2 and 1.3 in chapter 1 gives an introduction of the present research. The basic theories of nickel-base SC alloys, anisotropic elasticity, fracture mechanics, and finite element analysis are reviewed in chapter 2. The details of the FEM models, simulating a single-notch bar and its extension with a semi-elliptical crack embedded at the notch root are discussed in chapter 3. The numerical results are presented and discussed in chapter 4. Firstly, stress and strain concentration factors (SCF) of the notch bar are analyzed to characterize the notch effect on local stress and strain field, considering two typical material orientations, based on elastic-plastic material properties, with which material orientation dependence of the notch effect is analyzed and compared. In addition, the J integral, COD and CTOD of the semi-elliptical crack at the notch root are calculated respectively in two notch orientations. A variety of crack lengths and load levels are considered and discussed in order to investigate the material anisotropy effect on the crack front characteristic parameters.

Finally, from the results in chapter 4, a few conclusions on crack front characteristic parameters are obtained, and the suggested future work is described in chapter 5.

Chapter 2

Literature Review

2.1 Anisotropic Materials and SC Nickel-base Superalloys

2.1.1 Material Anisotropy

Generally speaking, anisotropy is a universal property of all crystalline materials, no matter whether single crystal or poly-crystal. The anisotropy of crystal shows as the dependence of physical properties on the crystallographic direction in which they are measured, such as electrical conductivity, thermal conductivity, thermal expansion coefficient, elastic modulus and strength. These anisotropic properties of crystal originate from the variation of atom packing along different lattice directions. But the anisotropic effects normally tend to be averaged out by the random arrangement of grains in polycrystalline materials, which are most widely used in practice. Therefore, the mechanical behaviour of the polycrystalline materials is usually based on isotropic assumption. However, apparent anisotropy may appear in a single crystal due to the regular atom packing throughout the grain, which usually leads to large variation of elastic-plastic properties in different material orientations, and plays a key role in small crack or anisotropic fracture analysis.

2.1.2 SC Nickel-base Superalloys

2.1.2.1 Development of SC Nickel-base Superalloys

Nickel-base superalloys have shown excellent high temperature strength, corrosion resistance and creep rupture strength that may satisfy the arduous operation condition of modern aircraft engine hot section [1]. The superior thermomechanical fatigue capabilities made them the ideal material for turbine hot section component application, as the maximum potential of the alloys may be exploited through optimized structure design. Today, nickel-base superalloys are increasingly being used as the material for the hot section components in engine propulsion system. In practice, the turbine blades and vanes are typically produced in SC form, whilst turbine discs in polycrystalline form.

SC nickel-base superalloys are formed with a high volume fraction of coherent intermetallic γ' precipitates dispersed throughout an austenitic face-centered cubic (FCC) nickel matrix [46]. The γ' precipitate also has an ordered face-centered cubic structure and works as the precipitation hardening constituent in nickel-base alloys. About ten different elements are generally used for alloying, with which some are used for specific purposes and others for multiple uses. A list of alloying compositions of some of the most common nickel-base SC superalloys is shown in Table 2.1. The development of SC superalloys has undergone three generations and fourth generation alloys are emerging. In Table 2.1, PWA 1480 from Pratt and Whitney was the first industrial SC superalloy to be used in civil aviation engines. The alloys CMSX-4, PWA 1484, Rene N5 and MC2 are

often labeled second generation. Characterized by very high temperature capabilities due to containing higher rhenium contents, CMSX-10 and Rene N6 are called third generation alloys with increased density. AM3, RR200 and CMSX-6 may be considered as a lower density compromise to the third generation alloys. CMSX-11B and CMSX-11C are specifically designed with high chromium to meet the hot corrosion and oxidation resistance requirements of land-based industrial turbine equipment.

2.1.2.2 SC Turbine Blade Manufacturing Technique

High temperature fractures of polycrystalline materials commonly occur intergranularly as a result of excessive precipitation, cavitation, and void formation at the grain boundaries that were oriented normally to the applied stress.

A turbine blade made of SC material eliminates the grain boundaries completely. Considering grain boundaries as weak points in the microstructure, the mechanical strength of the SC blade can be further increased [46]. In practice, the manufacturing of a SC nickel-base superalloy turbine blade combines the so-called “directional solidification” technique and grain selection technique. Directional solidification method is schematically shown in Figure 2.1(a) [47]. With carefully drawing the cooling mould out of the casting furnace into a liquid-cooled chamber, the crystal tends to extend along the entire length of the casting in columnar form. Thus the grain boundaries across the blade, perpendicular to the centrifugal tension in service, are eliminated. Generally, the grain growth direction is controlled in the desired preferential direction, which is corresponding to the optimum creep strength for cubic crystal dendrites [1]. When the

directional solidification technique is combined with a grain selector, the extra grains in directionally growing poly-crystal may be thoroughly eliminated and only one single grain is left through the whole width of the solidification front within the blade (Figure 2.1(b)). It should be noted that the terminology “single crystals” may only be considered to apply to the γ -nickel matrix for SC nickel base superalloy because of the presence of γ' precipitates as another phase. Since these γ' precipitates have little contribution to the global anisotropic properties, they are usually omitted in fracture analysis. The SC blades incorporating innovative cooling and coating designs can operate at gas path temperatures well above the melting point of the superalloy.

During the past fifty years, gas turbine engine performance has been greatly improved since the first generation due to two aspects of successful research, the achievements of increased turbine inlet temperature and decreased weight of turbine airfoils. Both of them are attributed to improvements in manufacturing techniques such as blade cooling, directional casting and SC technology, and application of thermal barrier coatings. Although investigations on fracture in SC superalloys have shown considerable practical significance in recent years [48-57], they are not sufficiently advanced to support the increasing application of the SC superalloys on hot section in high performance aircraft and rocket engines.

2.1.3 Direction Specification in Crystals

Considering a SC solid is formed by regularly stacking of millions of atoms, the identical packing feature may be discussed using a unit cell. Thus, any direction in the

unit cell may represent a certain direction in the crystal grain because a grain is simply the repeat of unit cells. As for FCC single crystal, the unit cell is schematically shown in Figure 2.2(a) and (b), and a material coordinate system is set up based on the three edges of the unit cell (Figure 2.2(c)), in which a direction can be specified with Miller indices [58] (Figure 2.2 (d)). Miller indices of direction gives a convenient way with which the feature of atom packing, or material anisotropic properties can be specified, and eventually unified with the crystal parameters. Miller indices of direction generally take the form as $[h \ k \ l]$. In a cubic symmetry system, the atom packing in directions of different Miller indices may be same, for example, $[110]$, $[101]$, and $[011]$ are all directions across the face diagonal of the cube, in which the atom packing shares identical features. These similar directions are usually grouped to a family of Miller indices and presented by only one of them. Thus, in considering anisotropic mechanical properties of a crystal solid, we can reasonably assume that they are identical in all directions that belong to the same Miller indices family. The significance of this assumption is that a certain problem in fracture analysis can be significantly simplified.

2.2 Theory of Anisotropic Elasticity

All formulae and definitions are considered in Cartesian coordinate system in this section unless it is otherwise specified.

2.2.1 Stress and Strain

When external force is applied to a solid body, the effects of this external force on any point inside the body may be expressed as the intensity of the internal reaction force on a unit surface where they act. This expression of internal forces is called stress. In the elasticity theory, the stress states at any point in a continuous solid body may be expressed as a stress tensor of rank two, which is often written in a matrix form [59] (Figure 2.3):

$$\sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix}. \quad (2.1)$$

The stress matrix is symmetrical with,

$$\begin{aligned} \sigma_{12} &= \sigma_{21}, \\ \sigma_{13} &= \sigma_{31}, \\ \sigma_{23} &= \sigma_{32}. \end{aligned} \quad (2.2)$$

Then only six independent components are left in the stress matrix, which can be simplified to an array:

$$\sigma = \begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{Bmatrix}. \quad (2.3)$$

Similarly, the displacement and distortion condition of any stressed point in a solid body is usually described in terms of strain, as:

$$\varepsilon = \begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \gamma_{23} \\ \gamma_{13} \\ \gamma_{12} \end{Bmatrix}. \quad (2.4)$$

Depending on the material properties such as elastic modulus, yielding strength and strain hardening reaction, stress and strain usually satisfy certain relationship that can be plotted as a typical stress-strain curve based on tensile test. The tensile test of anisotropic material may be carried out in several material orientations, in which the material behaves differently, then the apparent modulus in each orientation can be derived.

2.2.2 Generalized Hooke's Law

The linear strain-stress relationship for elastic body generally takes the form as

$$\varepsilon = \mathbf{S}\sigma, \quad (2.5)$$

where:

$$\mathbf{S} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ S_{21} & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ S_{31} & S_{32} & S_{33} & S_{34} & S_{35} & S_{36} \\ S_{41} & S_{42} & S_{43} & S_{44} & S_{45} & S_{46} \\ S_{51} & S_{52} & S_{53} & S_{54} & S_{55} & S_{56} \\ S_{61} & S_{62} & S_{63} & S_{64} & S_{65} & S_{66} \end{bmatrix}. \quad (2.6)$$

Equation (2.5) is called generalized Hooke's law [60].

The S_{ij} s in compliance matrix $\mathbf{S}$ may be either continuous or discontinuous variables for non-homogeneous body, or constants for homogeneous body. With matrix $\mathbf{S}$, each strain component may be expressed as a linear function of the corresponding stress components. From the material mechanics point of view, similar to Young's modulus and Poisson's ratio for isotropic elastic solid, the independent compliances in $\mathbf{S}$ matrix reflect the elastic mechanical properties of a certain material.

Sometimes it is convenient to express Generalized Hooke's law in stress-strain relationship as:

$$\sigma = C\varepsilon . \quad (2.7)$$

The so-called "Stiffness matrix" C is an inverse of compliance matrix S ,

$$C = S^{-1}. \quad (2.8)$$

Matrices S and C are fully symmetric along $i = j$ axis and the thirty-six compliances can be reduced to twenty independent constants [61]. To express the elastic mechanical properties of a fully anisotropic solid, the twenty material constants must be totally evaluated. Fortunately, crystal material usually possesses certain microstructure symmetry that can further reduce the number of independent terms in S or C matrix. For example, the stiffness matrix of orthotropic symmetric anisotropic material is expressed as:

$$C = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix}. \quad (2.9)$$

The number of independent elastic constants in equation (2.9) is 9.

For FCC SC superalloy which possess cubic symmetry, only three independent constants are left in the matrix as:

$$\begin{aligned} C_{11} &= C_{22} = C_{33}, \\ C_{44} &= C_{55} = C_{66}, \\ C_{12} &= C_{13} = C_{23}. \end{aligned} \quad (2.10)$$

All the other constants in the matrix are zero.

An ultimate simplification of the stiffness matrix is for isotropic materials, where only two independent constants are left. Since in engineering practice, Young's modulus E and Poisson's ratio ν are generally used parameters in fully defining stress-strain relationship, they can be transferred to matrix form as $\mathbf{S}$ or $\mathbf{C}$. The deployment of engineering constant E and ν to $\mathbf{C}$ for isotropic material is expressed in equation (2.11) [60].

$$\mathbf{C} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}(1-2\nu) & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}(1-2\nu) & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(1-2\nu) \end{bmatrix}. \quad (2.11)$$

2.2.3 Yielding Criteria of Isotropic and Anisotropic Materials

Generalized Hooke's law describes the elastic relationship between stress and strain, which results in the elastic material constants in engineering applications. However, most engineering materials have the ability to deform plastically. This ductile behaviour is generally expressed in certain yielding criteria, leading to another important material constant, the yielding strength. Two yielding criteria are commonly used for isotropic materials [62], Tresca maximum shear-stress criterion and Von Mises shear-strain energy criterion. The Von Mises criterion is expressed as:

$$2\sigma_s^2 = (\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2, \quad (2.12)$$

where σ_1, σ_2 and σ_3 are three principal stresses, and σ_s is the yielding strength of this material.

For an anisotropic solid body, the yielding behaviour is usually different in several material orientations, which leads to more complicated yielding criteria than in isotropic materials. To describe the yielding behaviour of an anisotropic material accurately and conveniently, a yield criterion may be expressed with mathematical equations that should not involve too many material parameters to be evaluated by experimental work.

In 1948, Hill [63] proposed a generalization of the Von Mises failure criterion named Hill's Potential Function. With six parameters characteristic of the anisotropic mechanical properties, which can be easily evaluated in simple tensile tests, Hill's Potential Function describes anisotropic material yielding behaviour with reasonable accuracy. Hill's potential function generally takes the following form:

$$2f(\sigma_{ij}) \equiv F(\sigma_{22} - \sigma_{33})^2 + G(\sigma_{33} - \sigma_{11})^2 + H(\sigma_{11} - \sigma_{22})^2 + 2L\sigma_{23}^2 + 2M\sigma_{31}^2 + 2N\sigma_{12}^2 = 1. \quad (2.13)$$

Hill's potential function is suitable for anisotropy with orthotropic symmetry where the three coordinate planes are the symmetry planes. In equation (2.13), σ_{ij} s are stress components defined in equation (2.1), while F , G , H , L , M , and N are anisotropic material parameters. All stress components are defined in the orthotropic symmetric Cartesian system, where three anisotropic principal axes are chosen as reference coordinates. For a material given the six material parameters, the yielding condition may be evaluated under any applied load by resolving the load in the above Cartesian system, then substitute the stress components into equation (2.13). Hill's potential function may not only be used as yielding criterion, but also enable a convenient way in defining anisotropic yielding behaviour of engineering materials. As an example, the calculation of the anisotropic material parameters, F , G , H , L , M , and N , is discussed in the ABAQUS manual and demonstrated in next chapter with PWA 1480 SC superalloy.

2.3 Fracture Mechanics

It is considered that all materials contain crack-like defects that constitute the nuclei of failure initiation in fracture mechanics. Thus fracture mechanics is applied in analyzing the load-bearing capacity of components with defects, or the fatigue crack propagation life of the components in service. Considering the loading applied on a cracked solid body, the crack may be stressed in three basic modes shown in Figure 2.4 [64]. The general case of loading condition can be well described by the superposition of the three modes. The loading of mode I is also known as the opening mode, which holds greater practical importance than the other two, sliding mode and tearing mode. Since high stress and strain occur in the vicinity of the defects as the driving force of crack propagation, the fracture analysis is generally concerned in the stress or strain field in such area.

Fracture mechanics involves two branches, LEFM and EPFM. LEFM has been well developed and widely applied in engineering fields, e.g. fatigue life prediction, while EPFM still has some difficulties and need further development.

2.3.1 Stress and Strain Concentration

Stress and strain concentrations are fillets, grooves, holes, notches, etc and may be found in most mechanical elements geometric discontinuities. The significance of these geometric discontinuities is that they usually cause the initiation of a crack. But the

analysis is more difficult because the elastic states within these areas are locally disturbed and this is addressed with stress (or strain) concentration factor, K_t (or K_ϵ) [64],

$$K_t = \frac{\sigma_{max}}{\sigma_{nom}}, \quad (2.14)$$

$$K_\epsilon = \frac{\epsilon_{max}}{\epsilon_{nom}}, \quad (2.15)$$

where the subscript “nom” represents stress or strain remote from the discontinuity and “max” represents stress or strain near the discontinuity. A schematic demonstration of stress concentration is shown in Figure 2.5, with the stress distribution in a notch area and the strain gradient at the notch root. The maximum tensile stress σ_{ymax} occurs at notch root and the nominal stress σ_{nom} is far from the notch area. Stress and strain concentration factors are considered material property dependent. If only elastic properties are assumed on the mechanical elements, $\sigma_{max}(\epsilon_{max})$ varies linearly with $\sigma_{nom}(\epsilon_{nom})$ when the geometry and the material properties of the elements have been defined, i.e., the stress and strain concentration factors are constants by definition. However, when plasticity is involved, stress concentration decreases, even disappears in fully plastic case, stress concentration factor is not applicable anymore because of non-linear behaviour of material after yielding. Ohgi *et al.* [38] reported the stress-strain distribution at notch root based on FEM results, which showed that the strain gradient in the notch root vicinity

was much larger than stress gradient under high tensile load because large plastic strain was introduced. The stress-strain gradient at notch root under elastic-plastic loading condition is schematically shown in Figure 2.6. However, strain concentration factors are still valid to show the influence of geometry discontinuity on local strain field. Different from the stress concentration factor in elastic elements, the strain concentration factor varies with different applied tensile loads in plastic elements and can reach very high level [65]. The investigation of strain concentration factor is significant for elastic-plastic fracture analysis. After yielding, the local stress concentration effect usually remains, but the strain concentration at the notch can be many times higher at high load level, which can eventually cause fracture long before local stress reaches the critical level.

Stress concentration factor reflects the stress state around some stress raiser, such as a notch. It becomes more serious as the notch radius is reduced. In the extreme condition that notch root radius approaches zero, a notch becomes a sharp crack, and the stress and strain becomes infinite at the crack tip in ideal elastic condition. From equations (2.14) and (2.15), stress and strain concentration factor become infinite, which is no longer applicable as the characteristic parameter of local stress field. Thus, another concept, stress intensity factor are introduced to describe the elastic stress state around cracks.

2.3.2 Characteristic Parameters of Crack Tip Stress-strain Field

2.3.2.1 The Limitation of Stress Intensity Factor

Stress intensity factor, the most important parameter in linear elastic fracture mechanics (LEFM), is based on the application of the theory of elasticity to continuum bodies containing cracks or defects. K depends on the far field boundary conditions and the geometry of the cracked solid. It expresses the strength of stress and strain fields near the crack tip.

In the mid-1950s, Irwin [66] pointed out that the local stresses in the neighborhood of the crack tip were of the general form:

$$\sigma_{ij} = \frac{K_I}{\sqrt{2\pi r}} f_{ij}(\theta) + \dots, \quad (2.16)$$

where K_I is the stress intensity factor for the loading condition of mode I, r and θ are cylindrical coordinates of a point with respect to the crack tip, while σ_{ij} is the stress components at this point, see Figure 2.7. Stress expressed in equation (2.16) shows inverse square root singularity when r approaches zero.

In LEFM region, K has received wide applications.

In the loading condition of mode I, crack length, applied load and K factor generally satisfy [64]:

$$K_I = F_{sn} \sigma \sqrt{\pi a} . \quad (2.17)$$

In equation (2.17), F_{sn} is a correction factor that depends on the boundary condition of the cracked body. SIF can be solved by analytical, experimental and numerical methods. In practice, the opening-mode SIF for 3D semi-elliptical crack takes the form as [67]:

$$K_I = F_{sn} \sigma \sqrt{\frac{\pi a}{Q}} , \quad (2.18)$$

where Q is defined as:

$$Q = E^2(k) \approx 1 + 1.46 \left(\frac{a}{c} \right)^{1.65} , \quad (2.19)$$

$$E(k) = \int_0^{\pi/2} \sqrt{1 - k^2 \sin^2 \phi} d\phi , \quad (2.20)$$

$$k^2 = 1 - \frac{a^2}{c^2} , \quad (2.21)$$

a and c are short and long semi-axes of the ellipse. ϕ is defined as elliptical angle.

Equation (2.17) is used to define an important fracture parameter, fracture toughness K_{IC} , also known as critical SIF. Fracture toughness may be considered as the fracture criterion in the material point of view. A crack is postulated to grow whenever the crack tip SIF K defined in equation (2.17) reaches K_{IC} . Fracture toughness of numerous engineering materials has been determined by experimental work in standard procedures described by American Society for Testing and Materials (ASTM) [68].

Stress intensity factor not only is a sufficient parameter to describe crack tip stress field for a steady crack, but it also plays a key role in fatigue crack life analysis. Many engineering problems have shown that the rate of fatigue crack propagation, da/dN , is governed by the stress intensity factor range ΔK [65]:

$$da/dN = f(\Delta K, R), \quad (2.22)$$

where

$$\Delta K = K_{max} - K_{min} = F_{sn} \Delta \sigma \sqrt{\pi a}, \quad (2.23)$$

$$\Delta \sigma = \sigma_{max} - \sigma_{min}, \quad (2.24)$$

$$R = \frac{\sigma_{min}}{\sigma_{max}}, \quad (2.25)$$

σ_{max} and σ_{min} represent maximum and minimum stress in a cyclic load pattern respectively, R is stress ratio.

In practice, since plastic deformation commences on most engineering materials when local yielding strength is reached, a plastic zone is generally considered existing instead of infinite stress at the crack tip. Irwin [3] estimated the size of the plastic zone and showed that the appearance of crack tip plastic zone makes the crack behave as if it were longer than its physical size. The effective crack length $a + r_p$ is known as Irwin's plastic zone correction (see Figure 2.8). Although plastic deformation is introduced into fracture analysis, Irwin's plastic zone correction may be considered as a simple extension of LEFM when moderate crack tip yielding occurs, where SIF still holds validity.

However, for short crack where crack tip plastic zone is large compared with crack size, Irwin's plastic zone correction cannot be applied any more. Given a for crack length and r_p for plastic zone radius, a general evaluation of the plastic zone in LEFM, or K validity is [15, 69]:

$$r_p \leq a/50. \quad (2.26)$$

The difficulties in the application of the LEFM method for short crack problems have emerged both from the evaluation of the propagation behaviour of short cracks themselves and in the transitional behaviour of such cracks as they grow from short to long cracks [4]. K cannot describe the stress field ahead of the crack tip with sufficient accuracy in the above conditions. The shortcomings of LEFM lie in its two basic assumptions:

- (1) The inelastic deformation in the vicinity of the crack tip is negligible, such that the crack responds elastically to the load. This assumption is valid when the crack length is much greater than the size of crack-tip plastic zone or for ideal brittle materials.
- (2) The material in crack-tip vicinity has general isotropy, such that crack responds independently to material orientations, which means as many as possible grains must be included in crack-tip zone.

These two assumptions are certainly invalid in the regime of short-crack growth where relatively large-scale plasticity occurs and local microstructural inhomogeneity may present accompanied by crystalline anisotropy. Also they are not applicable to cracks in single crystal superalloys. Since SIF in LEFM cannot satisfy the crack-tip solutions of the stress and strain distribution in the vicinity of short crack front, EPFM is applied, in which J integral and CTOD methods are generally used to solve elastic-plastic crack problems.

2.3.2.2 J Integral and CTOD

In 1968, Rice [70] gave the J integral expression for any 2D crack as:

$$J = \int_{\Gamma} (W dx_i - T_i \frac{\partial u_i}{\partial x_i} ds), \quad i = 1, 2. \quad (2.27)$$

The parameters in equation (2.27) are defined as:

Γ : an anticlockwise loop around crack tip that begins from under surface and ends at upper surface of a crack (Figure 2.9),

W : strain energy density of any point on the loop,

T_i : stress components of any point on the loop,

U_i : displacement components of any point on the loop.

Rice showed that J integral defined along any contour around the crack tip is path-independent, i.e., $J_{\Gamma_1} = J_{\Gamma_2}$ in Figure 2.9, and demonstrated the equivalence of J with the energy release rate and the proportionality of J with the CTOD.

Since J integral is the change in potential energy for a virtual crack extension da , given V as potential energy, the equivalence of J with the potential energy release rate G is demonstrated as:

$$J = -\frac{\partial V}{\partial a} = G \quad (2.28)$$

Thus J integral may be considered as the driving force of a crack extension. Since an integration loop can be taken far from the crack tip and then information about the crack tip can be deduced, it allows an extension of fracture mechanics from LEFM based on linear elastic assumption to EPFM involving elastic plastic behaviour. J integral,

similar as the role playing by K in linear elastic crack tip area, can describe the mean stress-strain field at the crack tip under elastic-plastic loading. Consider a material of which the stress-strain curve may be represented by an exponential function:

$$\sigma_e = A \varepsilon_{pe}^g, \quad (2.29)$$

stress and strain at a crack tip take the forms as[67]:

$$\sigma_{ij} = A \left(\frac{J}{A I_g} \right)^{\frac{g}{1+g}} \frac{1}{r^{\frac{g}{1+g}}} f_{ij}(\theta), \quad (2.30)$$

$$\varepsilon_{ij} = \left(\frac{J}{A I_g} \right)^{\frac{1}{1+g}} \frac{1}{r^{\frac{1}{1+g}}} \psi_{ij}(\theta), \quad (2.31)$$

where σ_e and ε_{pe} are equivalent stress and equivalent plastic strain respectively; A is correlation factor; g is hardening factor; I_g is a function of g and the loading mode, which equals 5 in tensile plain strain condition; $f_{ij}(\theta)$ and $\psi_{ij}(\theta)$ are position functions, which equal 1 when $i=j$ and 0 when $i \neq j$ respectively, in mode I loading condition.

In certain theoretical conditions, it has been shown by experiments that the governing equation for crack growth can be written as a function similar to Paris-Erdogan [71]:

$$da/dN = C(\Delta J)^m, \quad (2.32)$$

where ΔJ is the J integral range corresponding to the loading frame, and m is determined experimentally. It should be mentioned that the J integral method has strong analytical basis, which differs from the totally empirical Paris-Erdogan.

Also we can use J integral, usually written as J_{IC} , as the threshold of crack growth. The practical application of J depends on the possibility both to carry out the experimental procedure and to get the respective loading parameter for any geometry and loading condition. Some test standards for J_{IC} have been established by ASTM [72].

The use of J integral has some essential limitations in dealing with crack tip plasticity problems [64]. J integral, as a crack propagation control parameter, was proposed from energy approach, where the material behaviour was assumed nonlinear but elastic. However, the requirement of non-linear elastic stress-strain behaviour cannot be fulfilled in real material case, as unloading always follows a different path from loading curve (Figure 2.10), which is the reason why J integral can only be applied in monotonic loading conditions. For a propagating crack, some linear inelastic unloading always takes place in the wake of the new crack tip, which further limits the application of J within stationary crack problems.

As discussed above, a real crack in a solid body is generally 3D, and takes the form of a curved surface and crack front line. Crack may extend in any spatial direction at different rates because the driving force varies along crack front. This requires that the characteristic parameter of the crack tip stress field can be evaluated and is valid in 3D crack front. Although J integral proposed by Rice was for 2D crack in isotropic plates, it has been extended to 3D crack problems, for example, a semi-elliptical surface crack.

Considering a 3D crack with a tangentially continuous front, as shown in Figure 2.11, J integral may be defined as [73]:

$$\oint J(s) \delta \vec{a}(s) \vec{q}(s) ds = -\delta V . \quad (2.33)$$

Equation (2.33) is based on the virtual crack extension method, where δV is potential energy change corresponding to a $\delta \vec{a}$ crack increment in local crack extension direction $\vec{q}$. $J(s)$ is local average around point N. Local coordinate system is constructed with tangent $\vec{t}$ to the crack front at any crack front point N, the local direction of virtual crack extension $\vec{q}$ and the normal of the crack plane, $\vec{n}$. Thus the 2D J integral becomes a surface integral in 3D. In numerical software package ABAQUS, this surface integral finally substituted by volume integral around the crack front. As point N change positions, the J integral represents a pointwise energy release rate along the crack front.

The previous studies on J integral along a semi-elliptical surface crack front concentrated on geometry and loading conditions, for example, plate or pressurized cylinder conditions at different loading level [35-37, 39,45].

Yagawa *et al.* [35] analyzed the local J distribution for various configurations of semi-elliptical cracks in a plate subjected to uniform tension. It showed that the J distribution was affected by plate thickness, aspect ratio of semi-elliptical crack, material properties or loading conditions (tension or bending). Figure 2.12 is a diagram of normalized J integral distribution along the crack front from Yagawa's research, in which maximum local J integral occurred at about 60° position while minimum J integral on free surface, 90° position.

Wang [44] reported the similar J distribution for a 3D semi-elliptical surface crack on a plate under tension. Masahiko [39] investigated the J integral of a semi-elliptical crack in plate under bending condition (Figure 2.13), and reported the loss of path-independence of J integral in numerical results due to distorted mesh in this area. Yoon *et al.* [37] analyzed the semi-elliptical surface crack in a cylinder and determined the distribution of J integral of a 1/8 thickness flaw in a cylinder as shown in Figure 2.14, where maximum J occurred in 0° degree and minimum J in 90° position.

Ohgi *et al.* [38] analyzed the notch root semi-elliptical crack in FEM, and proposed the modification to an earlier conventional equation for estimating J integral values at two crack front positions. Ohgi's modification involves stress/strain gradient effect in the original equation, and obtained better correlation with the numerical results. The conventional equations from Ohgi showed that the J integral was controlled by the crack geometry and load level. Given same aspect ratio, J increased with crack size and applied load level.

Another approach to crack tip field analysis in EPFM is with the CTOD, a concept mostly based on a semi-empirical method. The basic idea of CTOD is that the crack-tip stress and strain field and hence the fracture behaviour of the cracked solid body may be controlled by a characteristic displacement at the crack tip. Thus, similar to J integral, CTOD can be considered a material constant to evaluate crack propagation threshold, $CTOD_{critical}$. However, because there is no natural displacement at the very crack tip [74], the limitation and practical difficulty of CTOD concept remains in its definition, which may vary in different problems. More than seven different definitions of the CTOD have been presented [75] since the first application of CTOD criterion, while a

unified CTOD that is applied like SIF in LEFM is still absent. Sometimes the CTOD measured at the intersection of the plastic boundary was considered [74,76,77] suitable for application. When fracture problems are analyzed in numerical methods, Rice's 90° intercept method (Figure 2.15) [39,70,75] is often used as an approach to extract CTOD from numerical results.

The theoretical definition of COD for 2-D crack in the case of LEFM may take the form as [64]:

$$\text{COD} = \frac{4\sigma}{E} \sqrt{a^2 - x^2}, \quad (2.34)$$

where E is Young's modulus and σ is nominal tensile stress.

By Irwin's plastic zone correction, the crack length was assumed to be $a + r_p$ (Figure 2.16). Applying this extended fictitious crack length in equation (2.34), an effective crack tip opening displacements may be given as,

$$\text{COD} = \frac{4\sigma}{E} \sqrt{(a + r_p)^2 - x^2}. \quad (2.35)$$

While $x = a$, by omitting the second order item r_p^2 ($a \gg r_p$), the crack opening displacement at crack tip is derived as:

$$\text{CTOD} = \frac{4\sigma}{E} \sqrt{2ar_p}. \quad (2.36)$$

In practice, equation (2.36) did not receive many applications in determination of CTOD, but it give a perfect demonstration of the essence of CTOD.

2.3.2.3 Relationships of CTOD, J and K

It turns out that CTOD, J integral and K can be related to each other under certain conditions from the energy point of view [64,67,75,78]. When LEFM applies, CTOD, J and K generally satisfy the following equations:

$$CTOD = \frac{K^2(1-\nu^2)}{E\lambda\sigma_s}, \quad (2.37)$$

$$J = K^2/E. \quad (2.38)$$

The value of λ in equation (2.37) depends on the position where the CTOD is measured. For quasi-elastic-plastic analyses, λ is usually between 1 and $4/\pi$.

In EPFM, CTOD and J integral relation is as follows:

$$J = n\sigma_s CTOD, \quad (2.39)$$

where n may be determined by experimental or numerical method [79]. The equivalence of J and CTOD as expressed in equation (2.39) denotes theoretically the application of CTOD as EPFM characteristic parameter of crack tip stress field.

2.4 FEM in Fracture Analysis

2.4.1 Significance of FEM in Fracture Analysis

The fundamental tasks in fracture analysis are to find either critical crack size or sub-critical fatigue crack growth life. Both types of analysis need the expression of the crack tip parameters mentioned above, such as K , J , or CTOD. These parameters may be evaluated analytically, experimentally and numerically according to different loading and structure conditions. Analytical method is the theoretical basis for the development of fracture mechanics, but usually it only works out with certain assumptions in order to simplify the problem, and large safety factors must be used in engineering applications. The shortcoming of experimental method lies to its restriction in laboratory environment. However, by the application of numerical method, there is almost no limit for an engineering problem, given enough computer resources. In practice, the emphasis in fracture analysis, especially in EPFM, has resorted to numerical method, for its great versatility in dealing with various engineering problems.

Numerical solutions are usually needed in both LEFM and EPFM crack analysis for several considerations:

- (1) The crack is located near complicated geometry area where stress concentration or complicated stress or strain distribution exists;
- (2) The cracks have irregular fronts in 3D state;
- (3) It is hard to find solutions by analytical and experimental methods, or numerical data are to be used to verify the experimental results for a fracture problem, in which analytical solution is unavailable.

With the robust capability of high-speed computers, elaborate numerical models for complicated engineering fracture problems may be simulated accurately. Ample research on fracture analysis has shown that numerical solution is able to provide accurate solution compared with analytical or experimental methods [36-41, 43-45, 75], and it is reliable in engineering applications.

2.4.2 FEM Technique in Fracture Analysis

The application of FEM in fracture mechanics lies in the mathematical description of a deformed solid based on continuum mechanics [80], in which stress and strain field can be derived based on equilibrium, compatibility, and constitutive equations, as well as stress-strain and strain-displacement relationships for specific boundary conditions. Since all the fracture parameters SIF, J integral and CTOD may be considered as continuum

mechanics quantities of a cracked solid body, they can be solved from displacement, strain and stress relationship.

Generally, finer mesh gives more accurate results in FEM analysis, but it leads to more costs and time. This contradiction may be solved with the following two techniques:

- (1) Using singular element in crack tip to model the crack tip singularity.
- (2) Using virtual crack extension to calculate energy release rates or J integral, usually in the domain integral method.

From equations (2-16) and (2-31), the strain (stress) singularity at the crack tip in a small-strain analysis is:

$$(1) \ \varepsilon \propto r^{-1/2} \text{ for linear elasticity, and}$$

$$(2) \ \varepsilon \propto r^{-1} \text{ for perfect plasticity.}$$

Including the singularity in finite element model improves the accuracy of the stress and strain calculation, and the characteristic parameters of stress field. The idea of singular elements was first proposed by Byskov [81], then a more elaborate singular element type was applied to model the appropriate stress (strain) singularity at crack tip

with singular elements for 2D (using 8-node second quadrilaterals), or 3D problem (using 20-node bricks) [82-84]. For example, in calculation of LEFM stress intensity factor, $r^{-1/2}$ singularity is obtained by using singular elements shown in Figure 2.17. For EPFM J integral, r^{-1} singularity may be obtained by leaving midside nodes of the adjacent sides at their original positions.

The second technique was first proposed by Hellen [85] in solving LEFM problems by FEM and Parks [86,87] extended it to accurately evaluate J integral for nonlinear elastic and elastic-plastic fracture problems. Shih *et al.* [88] further extended this method to evaluate 3D crack behaviour using FEM. Compared with some analytical solutions, K and J integral derived with such kinds of techniques provides excellent accuracy with rather coarse meshes [89]. ABAQUS package supports the contour integral in the domain integral method based on virtual crack extension technique, where 3D contour integral is extended to volume integral over a finite domain surrounding the crack front. The advantage of domain integral is that the errors of local solution have less effect on the global evaluated parameters, which consequently benefits the user with more accuracy and less costs.

Chapter 3

FEM Modeling

3.1 Anisotropic Material Constants of PWA 1480

The first industrial SC superalloy that has been used in civil aviation engines, Pratt and Whitney's PWA 1480, has a FCC crystal matrix. The mechanical properties of PWA 1480 have been investigated in detail and published in the experimental report by National Aeronautics and Space Administration (NASA) [90]. In this report, the apparent modulus, yielding and tensile strength, and creep properties of PWA 1480 in four lattice directions [001], [101], [213] and [111] were presented in a wide temperature range. As shown in the present FEM model, the typical anisotropic properties of PWA 1480 and adequate database make the material a good example for crack analysis of anisotropic materials. Considering the service condition of the fir-tree section of a turbine blade, the material and mechanical properties of PWA 1480 at 800°F (427°C) were selected (Table 3.1 and 3.2).

The experimental data of PWA 1480 in the tensile tests show that strain hardening effect of PWA1480 SC superalloy after yielding in all the four material orientations is very small at room temperature. Also at the high temperature, 650°C, strain hardening commences especially in [100] material orientation, but is not high over a large yielding region in the tensile curves. Thus a simplification of the material properties, perfect

plasticity in all material orientations was made for PWA 1480 SC superalloy in the present FEM model, as shown in Figure 3.1. As discussed in chapter 2, the definition of an anisotropic yielding behaviour is much more complicated than that of an isotropic yielding. In ABAQUS package, the definition of anisotropic yielding is based on Hill's potential function. To correlate PWA 1480 anisotropic tensile data with Hill's potential function constants, a series of mathematic calculations must be conducted.

3.1.1 Transformation of Stresses

A problem defined in one coordinate system x' , y' , and z' (prime) may be required to transfer to another coordinate system x , y , and z (original) (Figure 3.2). For example, the anisotropic mechanical properties of PWA1480 SC superalloy being considered in the present analysis must be referred to the material coordinate system first. Also, sometimes it is necessary to resolve the stress components to the material coordinates.

The transformation of stress component may be made in the transformation matrix method [60]:

$$\sigma = [Q]\sigma', \quad (3.1)$$

where σ and σ' are stress array in original and prime coordinate systems respectively.

The transformation matrix $[Q]$ takes the form as:

$$[Q] = \begin{bmatrix} \alpha_1^2 & \alpha_2^2 & \alpha_3^2 & 2\alpha_3\alpha_2 & 2\alpha_1\alpha_3 & 2\alpha_2\alpha_1 \\ \beta_1^2 & \beta_2^2 & \beta_3^2 & 2\beta_3\beta_2 & 2\beta_1\beta_3 & 2\beta_2\beta_1 \\ \gamma_1^2 & \gamma_2^2 & \gamma_3^2 & 2\gamma_3\gamma_2 & 2\gamma_1\gamma_3 & 2\gamma_2\gamma_1 \\ \beta_1\gamma_1 & \beta_2\gamma_2 & \beta_3\gamma_3 & (\beta_2\gamma_3 + \beta_3\gamma_2) & (\beta_1\gamma_3 + \beta_3\gamma_1) & (\beta_1\gamma_2 + \beta_2\gamma_1) \\ \gamma_1\alpha_1 & \gamma_2\alpha_2 & \gamma_3\alpha_3 & (\gamma_2\alpha_3 + \gamma_3\alpha_2) & (\gamma_1\alpha_3 + \gamma_3\alpha_1) & (\gamma_1\alpha_2 + \gamma_2\alpha_1) \\ \alpha_1\beta_1 & \alpha_2\beta_2 & \alpha_3\beta_3 & (\alpha_2\beta_3 + \alpha_3\beta_2) & (\alpha_1\beta_3 + \alpha_3\beta_1) & (\alpha_1\beta_2 + \alpha_2\beta_1) \end{bmatrix}. \quad (3.2)$$

All the items in [Q] are the direction cosines between the coordinate axes of the two coordinate systems, which are defined in Table 3.3.

Considering a cubic crystal loaded under a uniaxial tension in any [h k l] Miller indices of direction defined in the material coordinate system of x, y, z axes, and the only finite stress in any x', y', z' axes system is σ_x (i.e., $\sigma_y = \sigma_z = \sigma_{yz} = \sigma_{zx} = \sigma_{xy} = 0$). To transfer this σ_x to the material coordinate system, the direction cosines between the two coordinates are calculated firstly as:

$$\alpha_1 = h / \sqrt{h^2 + k^2 + l^2}, \quad (3.3)$$

$$\beta_1 = k / \sqrt{h^2 + k^2 + l^2}, \quad (3.4)$$

$$\gamma_1 = l / \sqrt{h^2 + k^2 + l^2}. \quad (3.5)$$

Then from equation (3.1), the stress components in the material coordinate system can be written as:

$$\sigma_x = \frac{h^2}{h^2 + k^2 + l^2} \sigma_x', \quad (3.6)$$

$$\sigma_y = \frac{k^2}{h^2 + k^2 + l^2} \sigma_x', \quad (3.7)$$

$$\sigma_z = \frac{l^2}{h^2 + k^2 + l^2} \sigma_x', \quad (3.8)$$

$$\sigma_{yz} = \frac{kl}{h^2 + k^2 + l^2} \sigma_x', \quad (3.9)$$

$$\sigma_{xz} = \frac{hl}{h^2 + k^2 + l^2} \sigma_x', \quad (3.10)$$

$$\sigma_{xy} = \frac{hk}{h^2 + k^2 + l^2} \sigma_x'. \quad (3.11)$$

Thus the tensile stress in any material directions of SC superalloy PWA 1480 may be resolved to the three material coordinates by using equations (3.6) - (3.11).

3.1.2 Yielding Strength Ratios in Hill's Potential Function

Hill's potential function may take the form as [89]:

$$f(\sigma) = \sqrt{F(\sigma_{22} - \sigma_{33})^2 + G(\sigma_{33} - \sigma_{11})^2 + H(\sigma_{11} - \sigma_{22})^2 + 2L\sigma_{23}^2 + 2M\sigma_{31}^2 + 2N\sigma_{12}^2}, \quad (3.12)$$

In equation (3.12), F, G, H, L, M, N are material constants defined as:

$$F = \frac{(\sigma^0)^2}{2} \left(\frac{1}{\sigma_{33}^2} + \frac{1}{\sigma_{22}^2} - \frac{1}{\sigma_{11}^2} \right) = \frac{1}{2} \left(\frac{1}{R_{33}^2} + \frac{1}{R_{22}^2} - \frac{1}{R_{11}^2} \right), \quad (3.13)$$

$$G = \frac{(\sigma^0)^2}{2} \left(\frac{1}{\sigma_{33}^2} + \frac{1}{\sigma_{11}^2} - \frac{1}{\sigma_{22}^2} \right) = \frac{1}{2} \left(\frac{1}{R_{33}^2} + \frac{1}{R_{11}^2} - \frac{1}{R_{22}^2} \right), \quad (3.14)$$

$$H = \frac{(\sigma^0)^2}{2} \left(\frac{1}{\sigma_{11}^2} + \frac{1}{\sigma_{22}^2} - \frac{1}{\sigma_{33}^2} \right) = \frac{1}{2} \left(\frac{1}{R_{11}^2} + \frac{1}{R_{22}^2} - \frac{1}{R_{33}^2} \right), \quad (3.15)$$

$$L = \frac{3}{2} \left(\frac{\tau^0}{\sigma_{23}} \right)^2 = \frac{3}{2R_{23}^2}, \quad (3.16)$$

$$M = \frac{3}{2} \left(\frac{\tau^0}{\sigma_{13}} \right)^2 = \frac{3}{2R_{13}^2}, \quad (3.17)$$

$$N = \frac{3}{2} \left(\frac{\tau^0}{\sigma_{12}} \right)^2 = \frac{3}{2R_{12}^2}, \quad (3.18)$$

where $\bar{\sigma}_{ij}$ is the experimental yield stress while σ_{ij} is applied as the only nonzero stress component; $f(\sigma)$ or σ^0 is the reference yield stress defined by the user. R_{ij} is anisotropic yield stress ratio, and $\tau^0 = \sigma^0 / \sqrt{3}$.

Hill's potential function provides a simple way in defining anisotropic yielding behaviour. The parameters F , G , H and L , M , N may be determined from simple tensile tests. The procedure is to get the yielding stress σ_s in x-direction firstly by tensile test, then substitute $\sigma_x = \sigma_s$ into Hill's potential function with all other stress components being zero. Thus we have

$$\sigma_s^2 = f^2(\sigma)/(G+H). \quad (3.19)$$

Given the yielding stress in other directions, we can solve the characteristic parameters by repeating the procedure of stress resolving, as discussed in section 3.1.1, and solving the set of equations.

PWA 1480 has a FCC crystal matrix that exhibits cubic symmetry (Figure 2.2), which can further simplify the current calculation. By defining the material coordinates in [100], [010] and [001] directions, it is reasonable to assume that:

$$\bar{\sigma}_{11} = \bar{\sigma}_{22} = \bar{\sigma}_{33}, \quad (3.20)$$

$$\bar{\sigma}_{12} = \bar{\sigma}_{23} = \bar{\sigma}_{13}. \quad (3.21)$$

Also the material constants in the symmetric directions are same:

$$F = G = H, \quad (3.22)$$

$$L = M = N. \quad (3.23)$$

Consequently we have,

$$R_{11} = R_{22} = R_{33}, \quad (3.24)$$

$$R_{23} = R_{13} = R_{12}. \quad (3.25)$$

By applying yielding stress in any two directions, we may get a set of material constants. It should be mentioned that the mathematical derivation based on different yielding directions does not result in an identical set of material constants H to N , as shown in Table 3.4. The changes of material constants originate from the tensile data in [123] direction that may lead to complete lose of real value solution as combined with [110] tensile data. This abnormal result may be due to two reasons. Firstly, Hill's potential function criterion is not a restricted mathematic expression for anisotropic yielding problems and the application of this yielding criterion has some limitations. Another reason is the error in tensile experiments. However, the combination of [100], [110], and [111] tensile data results in fairly stable material constants. The influence of [123] tensile data on yielding stress ratios, R_{ij} s, which are required in ABAQUS inputs, is

not significant. We can calculate the yielding stress ratio based on the average value of the material constants. With the reference yielding stress being equal to 989.4 MPa, the final results are evaluated as:

$$R_{11} = R_{22} = R_{33} = 0.9216, \quad (3.26)$$

$$R_{23} = R_{13} = R_{12} = 0.8853. \quad (3.27)$$

The calculation of the material constants and yielding stress ratio were carried out by a code written with MAT-LAB package (Appendix).

3.2 Description of the FEM Models

3.2.1 Definition of a Single-notch Bar

To investigate the strain concentration and crack behaviour at the notch root in a turbine airfoil made of PWA1480 single crystal, both loading condition and geometry in terms of material anisotropy have been taken into account in the present work. Figure 3.3 illustrates the so-called fir-tree attachment of turbine blades to the engine wheel rim and its loading condition. Since a SC turbine blade can be well controlled to grow in [001] orientation by using directional casting technique, a tensile load on the blade along [001] material orientation can simulate the actual centrifugal force applied to the blade in engine operating condition. To simplify the problem, the complicated geometry of a

turbine airfoil with the fir-tree blade attachment was reduced to a through-thickness single-notch bar, which is shown in Figure 3.4. The bar was assumed to have continuous and homogeneous anisotropic material properties.

Since geometry discontinuity (e.g. a notch or a crack) may initiate in any material direction, two material/notch orientations were considered in the present work with the material orientation indicated by the cubic material axes in a local material coordinate system (Figure 3.5), in which a uniaxial tensile load in the direction of the bar, i.e., $[001]$ material direction, is applied on the notch bar for both notch orientations.

- (1) With $[001]$ as the loading axis, the notch is in $[010]$ direction with its edge along $[100]$, it is named as $[001]/[100]$ orientation.
- (2) With $[001]$ as the loading axis, the notch is in $[\bar{1}10]$ direction with its edge along $[110]$, it is named as $[001]/[110]$ orientation.

3.2.2 FEM Model for Strain Concentration Analysis

For stress/strain concentration analysis, a FEM model of the SC single-notch bar, as shown in Figure 3.6, was created, using ABAQUS. Only half of the bar was meshed in order to save the computing cost due to geometry and loading symmetry, with twenty-node isoparametric brick elements. Finer meshes were used around the notch area. This model had a total of 680 elements with 4,872 nodes and 13,256 degrees of freedom.

3.2.3 FEM Model for Crack Analysis

Assuming that a semi-elliptical crack exists at the notch root, as schematically shown in Figure 3.7, three FEM meshes were created for the SC single-notch bar with cracks of the aspect ratio $a/c = 0.5$ and $c/d = 1/2, 1/3$ and $1/5$, which are named S1, S2 and S3 respectively. In the numerical analysis this cracked single-notch bar was simplified with considering only one fourth of the full model because of the loading and geometry symmetry. To achieve better solutions in the condition of large distortion in the notch-crack area that may occur due to large plastic deformation, much finer mesh was employed in the notch-crack area (Figure 3.8) than that in the model used for strain concentration analysis. This simplified notch-crack model was mainly constructed with 20-node quadratic brick elements, with some 15-node quadratic triangular prism elements in the transition areas. The total numbers of elements and nodes in S2 mesh are 24,610 and 105,013 respectively, and there are 315,039 degrees of freedom in total.

3.2.4 Displacement Controlled Load for FEM Model

Because the analyses involved nonlinear elastic-plastic deformation, the loading was implemented with displacement-control, in order to achieve a better convergence in the FEM runs. A series of end-displacements (0.1, 0.12, 0.15, 0.17, 0.2, 0.25, 0.3, 0.35, 0.4 mm in tensile direction) was chosen as the loading condition for strain concentration analysis, among which a subset (0.1, 0.2, 0.25, and 0.3 mm) was applied to the mesh S2, and only the 0.2 mm displacement was applied to S1 and S3 for fracture mechanics

analyses. For each of the loading conditions, two material orientations, as defined above, were considered.

Generally, the load level in a FEA model expressed in nominal stress is more straightforward and easier to discuss than applied surface displacement. It is also widely accepted in fracture analysis. Before any discussion of SCF, J and COD, it is necessary to evaluate the corresponding applied nominal stress to the control displacement. It was found that the material orientation and crack size had almost no influence on the applied nominal stress that was derived from each control displacement. Thus given the same control displacement, the corresponding applied nominal stress was considered same for all the three crack sizes, as well as for two notch orientations.

The investigation of the plastic zone size along the crack front under the 0.2 mm displacement load (nominal stress = 0.577 GPa) for the S1, S2, and S3 meshes showed that the plastic zone was fairly large compared with crack size, as shown in Figure 3.9 for the S2 mesh. The 0.2 mm load level can satisfy the elastic-plastic loading requirement of the present model.

Chapter 4

Results and Discussion

4.1 Strain Concentration Analysis for a Single-notch Bar

4.1.1 Model Consistency

Meshing technique is very important in finite element analysis because the element-size generally has a close relationship with the results. A general rule is to find suitable fineness of the mesh that can generate numerical results with acceptable accuracy. In strain concentration analysis, mesh around the notch area was refined gradually to get reasonable solutions with a representative case, e.g., the notched bar with the properties of an isotropic material of Young's modulus of 125 GPa and Poisson's ratio of 0.3, under axial load of 0.5 MPa, and the FEM mesh was refined until convergence less than 1% error was reached in the stress results. The numerical results with different mesh levels and tolerances between two immediate levels are shown in Table 4.1. The notch stress concentration factor was evaluated to be $K_t = 2.87$ within the elastic regime for the isotropic case. Theoretically, stress concentration factor does not vary with the magnitude of loading under elastic deformation. When the load level is decreased to 500 Pa, stress concentration factor is identical to the value obtained under the higher load level of 0.5 MPa in the current model. This verification proved that the 20

seeds (26 nodes along the notch curve) can provide accurate results for the current stress concentration analysis.

Because material anisotropy has been generally considered in the present analysis, it is necessary to investigate the anisotropic effect on the numerical solution. As discussed before, an isotropic material may be considered as the simplest anisotropic material, thus the above representative material with Young's modulus of 125 GPa and Poisson's ratio of 0.3, were transferred to matrix **C** form based on equation (2.11). The same result was obtained by using the anisotropic material model with its properties reducing to the above isotropic one, thus it was verified that the FEM model was valid for both isotropic and anisotropic cases.

4.1.2 Discussion of Stress and Strain Concentration

The strain concentration factor in the loading direction under each loading level was investigated. The numerical results of strain concentration are listed in Table 4.2. The nominal stress increase from 289 MPa to 849 MPa changes the notch area from fully elastic strain condition to large plastic strain condition. The plastic zone size according to different loading levels was shown in Figure 4.1 based on the FEM results.

The stress and strain gradient around the notch root in [001]/[100] notch orientation at the 578 MPa nominal stress level is plotted in Figure 4.2. In Y direction, both stress and strain increase rapidly from the edge of the notch area to a steady level around the center of the notch, but the gradient of strain is much larger than that of stress. In X direction, the stress and strain behave in different ways. Stress increases from notch

root to the peak value at about 0.5 mm depth under the notch surface, then decreases to a steady level. Strain shows the maximum magnitude at notch root and decreases rapidly to 0.5 mm depth under the notch surface, then approaches a steady level from there. Similar stress and strain distributions were obtained in [001]/[110] notch orientation. The distributions of the stress and strain in the current model agree with the analysis in previous publications [38,65] (Figure 2.6).

The relationship of strain concentration factor and load level is plotted in Figure 4.3 based on the data in table 4.2. It is found that no plastic strain was induced before the control displacement reaches 0.13 mm. The strain concentration factors in elastic region do not change with loading condition in both [001]/[100] (2.555) and [001]/[110] (2.405) notch orientations. However, once yielding commences, strain concentration factor increases rapidly with loading level. It should be mentioned that when material anisotropy is considered, as for any other parameters investigated in this research, strain concentration factor shows pronounced material orientation dependence, especially in small yielding condition. The strain concentration factor in [001]/100] is larger than that in [001]/110] notch orientation at each loading level, and the difference of strain concentration factor between two notch orientations varies from 6.2% in fully elastic region to 0.4% in large plastic region around notch area. A maximum 16% difference of strain concentration factor appears at the 720.9 MPa nominal stress level, which indicates that material anisotropy has great influence on strain concentration in the notch area in small scale yielding region. When large yielding occurs in the notch area, this orientation dependence of strain concentration factor nearly vanishes. The reason for the disappearance of the anisotropy effect on strain concentration factor is attributed to the

assumption of perfect plasticity, that is, an isotropic strain hardening method, for the PWA 1480 SC material.

4.2 Analysis of the Elastic-plastic Fracture Mechanics Parameters of the Semi-elliptical Surface Crack at the Notch Root

4.2.1 Numerical results of J Integral, COD, and CTOD along the Semi-elliptical Crack Front

With a semi-elliptical crack at notch root, J integral, COD and CTOD were evaluated respectively for each notch orientation under different loading condition. An isotropic material simplified from PWA 1480, with the properties of $E = 111\text{GPa}$, $\nu = 0.3$, $\sigma_y = 989.4\text{ MPa}$ and perfect plasticity strain hardening behaviour was applied on the S2 mesh under 0.557 GPa to verify the numerical model. The J integral variation along semi-elliptical crack front is investigated as a function of the particular elliptical angle ϕ as defined in Figure 4.4. The elliptical angle varies from 0° to 90° because of symmetry of the geometry. For each point at the crack front, three J integral paths were selected and the average was taken as the representative J integral value. It was found that the path-independence of J integral was preserved in the model with the difference less than 0.1-0.9% for the inner crack front, except that near the free surface area, i.e., point C in Figure 3.7 (b) (at $\phi = 90^\circ$ in Figure 4.4). The calculated J integral at point C did not have the path-independence with the maximum difference up to 45%. This

problem was of numerical modeling in nature perhaps due to large distortion of the deformed surface. It also has been reported in other studies on isotropic materials [39]. The numerical results of J integral are plotted in Figure 4.5-4.6. Figure 4.7 shows the crack size effect on J integral distribution along the crack front with three crack sizes in two notch orientations under the same loading level (nominal stress = 0.577 GPa). The J integrals at crack tip A, as shown in Figure 3.7(b), are plotted against crack size c in Figure 4.8. Figure 4.9 illustrates the variation of J integral with the load level for the S2 mesh at four crack front positions, where ϕ equals to 0° , 45° , 60° and 90° respectively.

Since for a semi-elliptical crack, the crack tip positions in elliptical axes, i.e. point A and C in the current model, may reflect the extreme influence of crack tip position on crack tip parameters, they are generally considered [38, 91, 92] in the relating analysis. In the current work, the COD is only calculated behind A and C crack front point, while the CTOD is extracted from the node displacement behind crack tip A using Rice's 90° intercept method [70]. The definition of COD and CTOD of both A and C crack front positions is shown in Figure 4.10. The COD with different crack sizes and load levels have similar profile as shown in Figure 4.11-4.14. The crack tip region is blunted by large plastic deformation, then the COD becomes smoothly increasing along the edge behind the crack tip. The CTOD and J integral of crack tip A are summarized in table 4.3-4.4. In each table, the difference of corresponding parameters between two notch orientations was calculated to show the material anisotropy effect.

The value of COD was calculated along the edge behind crack tip A and C, and the numerical results of the S2 mesh are plotted in Figure 4.15 and Figure 4.16 respectively. The numerical results of the COD of the S1 and S3 meshes under the 0.577

GPa nominal stress level are plotted in Figure 4.17 and Figure 4.18. The crack size effect on COD is demonstrated in Figure 4.19 and Figure 4.20 for each crack tip respectively.

4.2.2 Discussion of J Integral, COD, and CTOD

The previous research on semi-elliptical crack investigated the crack tip stress-strain field in consideration of several factors [35,39,44], such as the geometry of crack (crack front position, length and aspect ratio), the place where crack occurs (crack in plate, cylinder or at notch root), and load condition (load level and method). The crack front characteristic parameters may be influenced by any one of these factors or their combination. Therefore, the present discussion is divided into three aspects, considering crack front position, crack size, and applied load level effect respectively, with material orientation effect emphasized in each aspect.

4.2.2.1 J Integral Variation along Semi-elliptical Crack Front

The position effect originates from the essential 2D definition of both J integral and CTOD. In the previous research on semi-elliptical cracks, the position effect was usually demonstrated by plotting J integral along a semi-elliptical crack front (Figure 2.12-2.14). J variation along the crack front in isotropic materials and two notch orientations is compared in the present discussion. As shown in Figure 4.5(b), J variation in the isotropic notch bar is similar with the previous research on a semi-elliptical crack

in a tensioned plate [35]. Some difference around free surface region is due to the notch stress-strain concentration. J integral in the isotropic notch bar is generally larger than that in the anisotropic notch bar, with respectively 19% and 22% above that in [001]/[100] and [001]/[110] notch orientations in the anisotropic notch bar at 0° elliptical angle (point A). J integral variation along the crack front is very different between the two anisotropic notch orientations under elastic-plastic loading conditions. For example, in the [001]/[100] notch orientation of the S2 mesh under the 0.577 GPa nominal stress, J integral increases from 0° elliptical angle (point A) to the highest value at about 70° position, then decreases rapidly to the lowest value at point C, while in the [001]/[110] notch orientation, J integral decreases smoothly from 0° elliptical angle (point A) to about 60° position, then increases smoothly to 80° position, and finally decreases rapidly to the lowest value at free surface crack tip C. However, when the nominal stress reaches 0.825 GPa, large plastic deformation occurs along the crack front, the variation of J integral becomes close between the two notch orientations (Figure 4.5(d)). The J integrals in the [001]/[110] notch orientation are generally smaller than that in the [001]/[100] notch orientation at the same crack front position. No matter what load level or crack size, the minimum value of J integral along the semi-elliptical crack front occurs at the free surface, crack tip C.

It should be mentioned that the crack front position of the semi-elliptical crack also has effect on the COD distribution. From Figure 4.15-4.18, the variation of COD behind crack tip C is smoother than that behind crack tip A, while the blunt size of crack tip C is larger than that of crack tip A, for given same crack size and load level.

4.2.2.2 Crack Size Effect

Crack size has great influence on J integral along the crack front. From Figure 4.7, under the 0.577 GPa nominal stress, J integral along the crack front of the S1 mesh is much larger than that of S3 mesh, while J integral along the crack front of the S2 mesh is larger than that of S3 mesh and smaller than that of S1 mesh. Figure 4.8 shows that the J integral at point A increases with crack size. Similar trend of the J integral was also obtained by Hatanaka and Ohgi [38, 91, 92] for isotropic material at the two crack front positions, A and C. The crack size effect on J is different in two material orientations. The average differences of the J variation along the crack front between two cracks of S1, S2, and S3 in both notch orientations are shown in Table 4.5, the comparison between two notch orientations shows that the size sensitivity of the J integral along the crack front in [001]/[100] notch orientation is much higher than that in [001]/[110] notch orientation.

The crack size effect on the COD is plotted in Figure 4.19 and 4.20. It is shown that large-size cracks are usually accompanied by large crack tip blunting area for both crack tip A and C.

4.2.2.3 Load Level Effect

Load level effect on J integral is shown in Figure 4.9, where the tendency of J integral at four crack front positions of 0° , 45° , 60° and 90° for the S2 mesh is plotted against applied nominal stress in both notch orientations. It is deduced that J variation

along the crack front increases with load level. This conclusion is further verified by the elastic-plastic fracture model of through-the-thickness crack (2D) cracks in anisotropic materials proposed by Wu *et al.* [12] based on continuously distributed dislocation theory (CDDT), which theoretically expresses the energy release rate of a 2D crack in SC material under mode I loading condition as:

$$G = \frac{4a}{\pi} (t_2^F)^2 F_{22}^{-1} \ln \frac{c_2}{a}, \quad (4.1)$$

where F_{22} is a material constant calculated based on material stiffness matrix, c_2 is the parameter defining the range of the dislocation function, and

$$\ln \frac{c_2}{a} = \ln \left(\cos \frac{\pi t_2^0}{2t_2^F} \right)^{-1}. \quad (4.2)$$

In equations (4.1) and (4.2), a is crack length, $t_2^0 (= \sigma)$ is applied nominal stress and $t_2^F (= \sigma_s)$ is the yield strength in the tensile direction. The energy release rate G is equivalent to J integral. Under small-scale yielding condition, it reduces to

$$G = \frac{K^2}{2F_{22}}, \quad (4.3)$$

where K is the stress intensity factor for 2D crack in infinite media under uniform stress.

It may be of interest in engineering applications to correlate the energy release rate between a semi-elliptical crack and a through-the-thickness crack. To do this, we postulate that, at point A (0° elliptical angle), the semi-elliptical crack has the same SIF as that of a 2D crack that would have the size:

$$\bar{a} = a / Q, \quad (4.4)$$

where the factor Q is given in equation (2.19).

Considering the stress concentration of the current semi-elliptical crack embedded at the notch root, we can find a factor q to modify G of 2D crack in equation (4.1) for the current crack tip A by substituting K in equation (2.17) and equation (2.18) with stress concentration factor K_t (same value as the elastic SCF in table 4.2 for the current model) into equation (4.3) respectively, then comparing the corresponding G s.

$$q = (K_t)^2 / Q, \quad (4.5)$$

The modified energy release rate $\bar{G}$ (or analytical J integral) may be expressed as:

$$\bar{G} = \frac{4aq}{\pi} (t_2^F)^2 F_{22}^{-1} \ln \frac{c_2}{a}. \quad (4.6)$$

For crack tip A in the current cracked SC notch bar model of PWA1480 SC superalloys, F_{22}^{-1} equals 0.01123 GPa⁻¹ and 0.01019 GPa⁻¹, q equals 4.456 and 3.948 in

[001]/[100] and [001]/[110] notch orientations respectively, $a = 0.53$ mm and the yielding stress in tensile ([001]) direction is given in table 3.2. The results of $\bar{G}$ from equation (4.6) are listed in table 4.3 and plotted against normalized nominal stress in Figure 4.21. It is seen that the modified energy release rate $\bar{G}$ is in good agreement with the FEM calculated J integral for the semi-elliptical crack, when the load levels are not sufficiently high to cause excessive yielding over the entire cross-section. Deviation of $\bar{G}$ from FEM calculated J integral may be mainly attributed to two reasons: (1) the magnified (multiplied by the elastic stress/strain concentration factor) stress employed in calculating $\bar{G}$ represents a higher stress state than the real stress distribution in front of the notch, the latter decreases as the distance from the notch root increases, therefore, this causes higher-values of $\bar{G}$ than FEM calculated J under small scale yielding conditions, even though the difference appears to be small in this region; (2) the modification of G is based on small-scale yielding condition, when large yielding occurs along crack front, q becomes invalid, plus when the yielding scale approach to covering the entire cross-section, the effect of finite geometry may play a significant role, when σ/σ_s is greater than 0.7, the difference becomes increasingly large.

Since J integral and CTOD may be theoretically represented as the energy release rate, as expressed in equation (2.28) and (2.39), the material orientation dependence of both J integral and CTOD at crack tip A in the present model may be reasonably explained using equation (4.1). The item F_{22}^{-1} in equation (4.1), as the representation of the material orientation dependence of G , is larger in [001]/[100] notch orientation than

that in [001]/[110] notch orientation, and consequently leads to larger G (or J , CTOD) in [001]/[100] notch orientation.

The load level effect on COD is demonstrated in Figure 4.11 - Figure 4.14. It can be seen that higher load usually results in larger COD. Figure 4.15-Figure 4.18 shows that the COD in [001]/[100] notch orientation is always larger than that in [001]/[110] notch orientation for same crack size and loading level. The material orientation effect on COD is obvious along the distance from either the crack tip A or C, and the difference of COD between the two orientations steadily maintained at 10% for different crack sizes. However, under higher load level, such as the 0.825 GPa nominal stress, it drops significantly to 5% for the S2 mesh.

4.2.3 Evaluation of EPFM Parameter n between J and CTOD

CTODs and corresponding J integral values of crack tip A in Table 4.3 and 4.4 show that they have similar orientation dependence. Both of them increase with the crack size at same loading level, and with the load level for the same crack size. The anisotropy effect on J and CTOD is most significant for the small crack of the S3 mesh compared with other crack sizes, or under the 0.719 GPa nominal stress when the load level effect is considered for the same crack size. Since CTOD and J satisfy certain relationship as discussed in equation (2.39), the relationship between J and CTOD of crack tip A was examined for all evaluated cases in the current fracture analysis similarly to isotropic materials, with the yielding stress equaling 989.4 MPa (in tensile direction). The correlation number n is listed in table 4.6 for all the evaluated cases. The average n

between two notch orientations shows less than 6% difference. Theoretically, according to Irwin's closure integral, $n = 1$. However, due to the definition of CTOD in the numerical analysis, which was taken at some distance behind the crack tip, n is generally less than 1.

Chapter 5

Conclusions

5.1 Single-notch Bar Model

- The stress and strain distributions in the notch area were calculated, and agreed with the published research. The stress (or strain) concentration factors do not change with applied load within elastic deformation region, while the strain concentration factors increase with applied load in two notch orientations in elastic-plastic deformation region.
- The material anisotropy effect on stress and strain concentration was investigated. It is shown that material anisotropy has great influence on stress and strain concentration for the PWA 1480 SC single-notch bar especially in small yielding notch area. The maximum difference of strain concentration factor between [001]/[100] and [001]/[110] notch orientations was found to be 16%.

5.2 Cracked Single-notch Bar Model

- The J integral along a semi-elliptical crack embedded at the notch root was evaluated at different loading levels and for several crack sizes. It was found that the J integral varied along the semi-elliptical crack front, and the distribution of

the J integral was influenced by the crack size, load level and material anisotropy. The minimum J integral was found at the free surface of the crack front. Material anisotropy had influence on the J integral distribution. The J integrals in the [001]/[100] notch orientation are generally larger than those in the [001]/[110] notch orientation.

- The CODs of two typical crack front positions, A and C, which are in the short and long semi-axes respectively, were evaluated and also compared. The COD increases much faster in the vicinity of the crack tip for the plastic deformation, which consequently causes the crack blunt, then approaches smoothly increasing along the edge behind the crack tip. The COD at point C is larger than that at point A independent of crack size or loading level. Both crack size and loading level had positive influence on the COD. The COD in the [001]/[100] notch orientation are larger than that in the [001]/[110] notch orientation. The material anisotropy effect on the COD is pronounced in small-scale yielding condition, while decreases when large crack tip yielding occurs.
- The J integral at crack tip A increases with crack size, which is similar to the trend obtained in a published conventional model of J calculation of the notch root semi-elliptical crack. The size sensitivity of the J integral along the crack front in the [001]/[100] notch orientation is much higher than that in the [001]/[110] notch orientation.
- The load level and material anisotropy effects on the J integral and CTOD at crack tip A were correlated to a published anisotropic fracture model for a 2D crack in SC materials. The modified energy release rate $\bar{G}$ from the analytical

model is in good agreement with the current FEM calculated energy release rate for the semi-elliptical crack, when the load levels are not high enough to cause excessive yielding over the entire cross-section at notch root.

- It was found that the influences of material anisotropy on the J integral and CTOD of crack tip A were different. The relationship between J and CTOD of crack tip A was examined similarly to isotropic materials. The correlation number n between J and CTOD was found less than 1.

5.3 Suggested Future Work

- The anisotropic plastic hardening properties of SC materials may be taken into account in the finite element model of fracture analysis, as well as the creep behaviour of the SC superalloys in elevated temperature condition for real turbine airfoils. Thus the material orientation effects on the SCF and the J variation along the semi-elliptical front, as well as CTOD may be evaluated in large-scale yielding region.
- Different aspect ratios should be considered with more crack sizes and load levels in the FEM analysis to obtain more detailed data which can be used as estimation control or verification of similar crack geometry in the fatigue crack experiments.
- The semi-elliptical crack evaluation in plates may be carried out for similar anisotropic materials to investigate the material anisotropy effects on crack behaviour, the stress and strain field at the crack front, with which analytical verification is relatively easier and the numerical data should be more applicable

for the derivation of small crack fracture models, from material anisotropy point of view.

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Table 2.1 Compositions of the most common nickel-base SC superalloys [46].

Alloy	Ni	Cr	Co	Mo	W	Al	Ti	Ta	Re	Nb	V	Hf
PWA 1480	62.5	10	5		4	5	1.5	12				
Rene N4	62.6	9	8	2	6	3.7	4.2	4		0.5		
CMSX-2	66.6	8	4.6	0.6	7.9	5.6	0.9	5.8				
SRR99	66.5	8.5	5		9.5	5.5	2.2	2.8				
AM1	63.8	7.8	6.5	2	5.7	5.2	1.1	7.9				
CMSX-11B	62.1	12.5	7	0.5	5	3.6	4.2	5		0.1		0.04
CMSX-11C	64.5	14.9	3	0.4	4.5	3.4	4.2	5		0.1		0.04
MC2	64.5	8	5	2	8	5	1.5	6				
CMXS-4	61.8	6.5	9	0.6	6	5.6	1	6.5	3			0.1
PWA1484	59.4	5	10	2	6	5.6		9	3			
RENE N5	61.8	7	8	2	5	6.2		7	3			0.2
CMSX-10	69.6	2	3	0.4	5	5.7	0.2	8	6	0.1		0.03
RENE N6	57.4	4.2	12.5	1.4	6	5.75		7.2	5.4			0.15
RR2000	61.5	10	15	3		5.5	4				1	
AM3	67.7	8	5.5	2.25	5	6	2	3.5				
CMSX-6	70.4	10	5	3		4.8	4.7	2				0.1

Table 3.1 Elastic constants of PWA 1480 at 800°F (427°C).

	C_{1111}	C_{1122}	C_{2323}
Unit (Msi)	34.1	22.6	16.9
Unit (GPa)	235.2	155.9	116.6

Table 3.2 Mechanical properties of PWA 1480 at 800°F (427°C).

Direction	[100]	[110]	[111]	[123]
0.2% Yielding (MPa)	989.4	921.9	897.0	837.7
Tensile Strength (MPa)	1118.4	957.0	1393.5	1218.3
Apparent Modulus (GPa)	111.0	206.2	289.0	206.2

Table 3.3 Direction Cosines of two coordinate systems.

	x	y	z
x'	α_1	β_1	γ_1
y'	α_2	β_2	γ_2
z'	α_3	β_3	γ_3

Table 3.4 Yielding strength ratios and material constants based on the test data in different orientations.

Loading Direction 1	Loading Direction 2	σ^0 (MPa)	R_{11}	R_{12}	F, G, H	L, M, N
[1 0 0]	[1 1 0]	989.4	1	0.912	0.5	1.8036
[1 0 0]	[1 1 1]	989.4	1	0.9066	0.5	1.8249
[1 0 0]	[1 2 3]	989.4	1	0.8093	0.5	2.29
[1 1 0]	[1 1 1]	989.4	1.0221	0.9066	0.4786	1.8249
[1 1 0]	[1 2 3]	989.4	Unavailable			
[1 1 1]	[1 2 3]	989.4	0.7198	0.9066	0.965	1.8249

Table 4.1 Mesh refinement around the notch area.

Mesh level	Seeds number along the notch	Maximum stress in loading direction in the notch area (MPa)	Difference between two sequential meshes
1	5	1.635	
2	10	1.336	22%
3	15	1.419	6%
4	20	1.436	1%

Table 4.2 Strain concentration factors of the PWA 1480 single notch bar.

Control displacement (mm)	Nominal Strain (10^{-3} mm/mm)	[001]/[100] notch orientation				[001]/[110] notch orientation			Difference of SCF
		Nominal stress (GPa)	Max. strain (10^{-3} mm/mm)	SCF		Nominal Stress (GPa)	Max. strain (10^{-3} mm/mm)	SCF	
0.1	2.6247	0.289	6.707	2.555		0.289	6.312	2.405	6.2%
0.12	3.1496	0.347	8.048	2.555		0.347	7.574	2.405	6.2%
0.15	3.9370	0.434	10.41	2.644		0.434	9.311	2.365	11.8%
0.17	4.4619	0.491	12.68	2.842		0.492	11.26	2.524	12.6%
0.2	5.2493	0.578	17.25	3.286		0.578	15.07	2.871	14.5%
0.25	6.5617	0.721	28.92	4.407		0.721	24.94	3.801	16%
0.3	7.8740	0.835	69.48	8.824		0.836	66.06	8.390	5.1%
0.35	9.1864	0.847	169.3	18.429		0.847	167.7	18.255	1.0%
0.4	10.4987	0.849	271.0	25.813		0.849	270.0	25.717	0.4%

Table 4.3 CTOD, J integral and $\bar{G}$ at crack tip A of the S2 mesh at different load levels.

Nominal stress (Gpa)	[001]/[100]			[001]/[110]			Difference		
	CTOD (μ m)	J (KN/m)	$\bar{G}$ (KN/m)	CTOD (μ m)	J (KN/m)	$\bar{G}$ (KN/m)	CTOD	J	$\bar{G}$
0.289	3.566	2.570	3.610	3.206	2.489	2.902	11%	3%	19.6%
0.577	15.223	12.560	16.396	13.566	12.099	13.182	12%	4%	19.6%
0.719	30.114	25.621	28.974	26.791	23.899	23.294	12%	7%	19.6%
0.825	86.750	75.560	44.778	81.968	72.251	35.999	6%	5%	19.6%

Table 4.4 CTOD and J integral at crack tip A under the nominal stress of 0.577 GPa.

Crack size (mm)	Notch orientation [001]/[100]		Notch orientation [001]/[110]		Difference	
	CTOD (μ m)	J (KN/m)	CTOD (μ m)	J (KN/m)	CTOD	J
S1 ($2c=3.175$ mm)	16.585	14.155	15.149	13.658	9%	4%
S2 ($2c=2.117$ mm)	15.223	12.560	13.566	12.099	12%	4%
S3 ($2c=1.270$ mm)	12.341	9.503	10.951	8.947	13%	6%

Table 4.5 Comparison of crack size effect on J between two notch orientations.

<div><div>Difference</div><div>Crack Size</div></div>	Difference of J between two crack fronts (N/m)		Difference of size effect between two notch orientations
	Notch orientation		
	[001]/[100]	[001]/[110]	
S1 vs. S2	1830	1521	20%
S1 vs. S3	5614	4759	18%
S2 vs. S3	3784	3238	17%

Table 4.6 Derivation of n from J and CTOD.

Crack size	Notch orientation	Nominal stress (GPa)	CTOD (μm)	σ_s (MPa)	n	J integral (N/m)	Average n	
							[001]/[100]	[001]/[110]
S1	[001]/[100]	0.577	16.585	989.4	0.86	14155	0.82	0.87
	[001]/[110]		15.149	989.4	0.91	13658.3		
S2	[001]/[100]	0.289	3.566	989.4	0.73	2569.594		
		0.577	15.223		0.83	12559.893		
		0.718	30.114		0.86	25620.641		
		0.825	86.750		0.88	75560.23		
	[001]/[110]	0.289	3.206	989.4	0.78	2488.512		
		0.577	13.566		0.90	12099.317		
		0.718	26.791		0.90	23899.172		
		0.825	81.968		0.89	72250.909		
S3	[001]/[100]	0.577	12.341	989.4	0.78	9503		
	[001]/[110]		10.951	989.4	0.83	8947

Figure 1.1 Turbine blade (RB211 HP turbine blade) [1].

Figure 1.2 Crack regions defined by Kitagawa-Takahashi curve [5], where σ_{cy} is the cyclic yield stress in a reversed stress test, and l represents the limit of crack length beyond which LEFM is valid.

(a) Directional solidification [47]

(b) A turbine blade with grain selector in position

Figure 2.1 SC blade casting techniques.

(a) Solid sphere model of FCC matrix

(b) FCC unit cell model

(c) Material coordinate system based on unit cell

(d) Miller indices of direction [58]

Figure 2.2 FCC single crystal matrix and Miller indices.

Figure 2.3 Stress components.

Figure 2.4 Three loading modes [64] .

Figure 2.5 Elastic strain and stress gradient in the notch region.

Figure 2.6 Plastic strain and stress gradient in the notch region [65].

Figure 2.7 Definition of crack tip stress intensity factor.

Figure 2.8 Irwin's plastic zone correction [3].

Figure 2.9 Contours around the crack tip.

Figure 2.10 Unloading behaviour of materials.

(a) Virtual crack extension in a 3D crack front

(b) General mesh in FEM model and COD behind crack tip node set N (in section A-A)

Figure 2.11 Definition of 3D J integral and COD along 2D crack front.

Figure 2.12 Local J integral variation along the crack front in a plate under tension (aspect ratio $a/t = 0.8$, $a/c = 0.6$) [35].

Figure 2.13 Local J integral variation along the crack front in a plate under bending (aspect ratio $a/t = 0.42$, $a/c = 0.2$) [39].

Figure 2.14 J integral variation along the crack front of a cylinder surface flaw [37].

Figure 2.15 Definition of CTOD: the 90 o interception method by Rice.

Figure 2.16 Definition of COD and CTOD [64].

Figure. 2.17 Crack tip singular elements in 2D and 3D models.

(a) Tensile curves at room temperature

(b) Tensile curves at 650° C

Figure 3.1 Perfect plasticity simulation of PWA 1480 [90].

Figure 3.2 Two coordinate systems.

Figure 3.3 Loading conditions of a turbine blade.

Figure 3.4 Dimensions of single-notch bar model.

Figure 3.5 Notch orientations defined in local material coordinate system.

Figure 3.6 Mesh of half the single-notch bar.

Figure 3.7 Semi-elliptical crack embedded at the notch root.

Figure 3.8 Mesh of one-fourth of the notch bar with a semi-elliptical crack.

Figure 3.9 Plastic strain distribution at the crack front.

(a) Nominal stress = 0.289 GPa

(b) Nominal stress = 0.578 GPa

(c) Nominal stress = 0.835 GPa

Figure 4.1 Yielding regions under different load levels.

(a) Stress and strain gradients along the notch edge

(b) Stress and strain gradient in the notch direction

Figure 4.2 Stress and strain gradients in the notch region.

Figure 4.3 Strain concentration factors at different loading levels.

Figure 4.4 Definition of the elliptical angle for the semi-elliptical crack front.

(a) Nominal stress = 0.289 GPa

(b) Nominal stress = 0.577 GPa

(c) Nominal stress = 0.718 GPa

(d) Nominal stress = 0.825 GPa

Figure 4.5 J variation along the S2 crack front.

(a) S1 mesh

(b) S3 mesh

Figure 4.6 J variation along the crack front of the S1 and S3 meshes (nominal stress = 0.577 GPa).

(a) [001]/[100] notch orientation

(b) [001]/[110] notch orientation

Figure 4.7 Crack size effect on J integral (nominal stress = 0.577 GPa). Figure 4.8 Crack size effect on J integral at crack tip A (nominal stress = 0.577 GPa).

(a) [001]/[100] notch orientation

(b) [001]/[110] notch orientation

Figure 4.9 Load level effect on J of the S2 mesh.

Tension direction
[001]

1/2 COD

1/2 CTOD Blunt area

(a) Behind crack tip C

Tension direction
[001]

(b) Behind crack tip A

Figure 4.10 Definition of COD and CTOD.

(a) Nominal stress = 0.289 GPa

(b) Nominal stress = 0.577 GPa

(c) Nominal stress = 0.718 GPa

(d) Nominal stress = 0.825 GPa

Figure 4.11 COD profile behind crack tip A of the S2 mesh under each load level.

(a) Nominal stress = 0.289 GPa

(b) Nominal stress = 0.577 GPa

(c) Nominal stress = 0.718 GPa

(d) Nominal stress = 0.825 GPa

Figure 4.12 COD profile behind crack tip C of the S2 mesh under each load level.

(a) S1 mesh

(b) S3 mesh

Figure 4.13 COD profile behind crack tip A of the S1 and S3 meshes
(nominal stress = 0.577 GPa).

(a) S1 mesh

(b) S3 mesh

Figure 4.14 COD profile behind crack tip C of the S1 and S3 meshes
(nominal stress = 0.577 GPa).

(a) Nominal stress = 0.289 GPa

(b) Nominal stress = 0.577 GPa

(c) Nominal stress = 0.718 GPa

(d) Nominal stress = 0.825 GPa

Figure 4.15 COD behind crack tip A of the S2 mesh.

(a) Nominal stress = 0.289 GPa

(b) Nominal stress = 0.577 GPa

(c) Nominal stress = 0.718 GPa

(d) Nominal stress = 0.825 GPa

Figure 4.16 COD behind crack tip C of the S2 mesh.

(a) S1 mesh

(b) S3 mesh

Figure 4.17 COD behind crack tip A of the S1 and S3 meshes (nominal stress = 0.577 GPa) .

(a) S1 mesh

(c) S3 mesh

Figure 4.18 COD behind crack tip C of the S1 and S3 meshes (nominal stress = 0.577 GPa).

(a) [001]/[100] notch orientation

(b) [001]/[110] notch orientation

Figure 4.19 Crack size effect on the COD behind crack tip A.

(a) [001]/[100] notch orientation

(b) [001]/[110] notch orientation

Figure 4.20 Crack size effect on the COD behind crack tip C.

Figure 4.21 Correlation of J integral values from FEM analysis and Wu's analytical model (at crack tip A of the S2 mesh) [12].

Appendix

Matlab code for yielding stress ratio calculation.

```
% This program is to calculate the six(two) yield stress ratios of FCC single crystal as
input in
% ABAQUS software for anisotropic yielding definition based on Hill's potential
function.
% The tensile strength in any [h k l] material direction are found through uniaxial tensile
tests.
% date      Version      programmer
% Jan03 03   original     Jun Zhao
% variables definition:
% i-----count of the loading direction
% thigma----yielding strength from tensile test
% h,k,l----loading direction in material coordinate system
% arfa-----direction cosine of loading direction with x-direction
% beta-----direction cosine of loading direction with y-direction
% gama-----direction cosine of loading direction with z-direction
% thigma11,22,33,23,13,12----stress components of thigma in xyz system
% thigma00----reference yielding strength
% a11,a12,a21,a22,b1,b2----constants in linear equations of material constants
fgh,lmn
% fgh, lmn-----material constants
% r1,r2----R11=R22=R33=r1; R12=R13=R23=r2
% A, B----- linear equation matrix
% material_const----material matrix,[fgh lmn]
% The unit for yielding strength thigma is Pa
clear
i=1;
while i<=2
    % Promote the user to input loading direction
    h=input('enter h:');
    k=input('enter k:');
    l=input('enter l:');
    %Promote the user to input tensile strength
    thigma=input('enter the yielding strength value in Pa:');
    %Promote the user to input reference yielding strength
    thigma00=input('enter the reference yielding strength value in Pa:');
    arfa=h/(h^2+k^2+l^2)^(1/2);
```

```

beta=k/(h^2+k^2+l^2)^(1/2);
gama=l/(h^2+k^2+l^2)^(1/2);
thigma11=thigma*arfa^2;
thigma22=thigma*beta^2;
thigma33=thigma*gama^2;
thigma23=thigma*beta*gama;
thigma13=thigma*arfa*gama;
thigma12=thigma*arfa*beta;
if i==1
    a11=2*(thigma11^2+thigma22^2+thigma33^2-thigma11*thigma22-
thigma11*thigma33-thigma22*thigma33)
    a12=2*(thigma23^2+thigma13^2+thigma12^2)
    b1=thigma00^2;
else
    a21=2*(thigma11^2+thigma22^2+thigma33^2-thigma11*thigma22-
thigma11*thigma33-thigma22*thigma33)
    a22=2*(thigma23^2+thigma13^2+thigma12^2)
    b2=thigma00^2;
end
i=i+1;
end
A=[a11 a12;a21 a22];
B=[b1;b2];
material_const=A\B;
fgh=material_const(1,1)
lmn=material_const(2,1)
r1=(1/(2*fgh))^(1/2)
r2=(3/(2*lmn))^(1/2)
% end of the program

```