

文章编号: 1000-8055(2012)12-2778-08

Fatigue-crack-initiation numerical modelling of a Ni-base powder metallurgy alloy

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Abstract: A simplified three-dimensional numerical model was presented to simulate the micro-crack nucleation and growth to some predefined dimension (approximately 0.38 mm) on the throat surface of a Ni-base powder metallurgy (PM) specimen. The numerical simulation of micro-crack initiation was based on the Tanaka-Mura micro-crack initiation models, where individual grains of the mesoscopic model were simulated using the Voronoi tessellation. Four improvements were made in the model. (1) Considering crack initiation along with 12 principal slip systems on octahedral slip planes of face centered cubic (FCC) crystal in three-dimensional (3-D) models. (2) Considering the effect of secondary phase precipitate due to impinging slip and dislocation pileup. (3) The Tanaka-Mura theory of fatigue-crack-initiation from notches was applied to simulate the crack initiation from another crack tip. (4) The coalescence of random initiated micro-cracks was simulated once they intersected with each other and a macro-crack was finally formed. The calculated results were in good agreement with the experimental data which verified the rationality of the simulation model. The applicability of the proposed model for treating fatigue-crack-initiation life in engineering structures was preliminarily achieved.

Key words: fatigue-crack-initiation; numerical simulation; slip system; powder metallurgy; Voronoi tessellation

CLC number: V232.3

Document code: A

Fatigue in engineering structures involves crack initiation and growth process. Current life prediction approaches for gas turbine deal with both crack initiation and propagation lives. Typically, a gas turbine component is designed to have a minimum low cycle fatigue (LCF) crack initiation life exceeding the specified service life and a crack propagation life from an assumed initial inspection interval that is twice the number of service cycles between inspections^[1]. The current life prediction methods based on phenomenological theories, are expensive to establish, because a large amount of experimental databases are required. The current life prediction systems may be improved by development of better fatigue-crack-initiation models, based on

the crystalline microstructure simulation.

Fatigue-crack-initiation life typically refers to formation and growth of micro-cracks to some predefined dimensions, often based on microstructure scales, on the order of 50—500 μm ^[2]. At the length scale of grains, fatigue crack nucleation and growth depended crucially on microstructural features such as grain size, crystallographic orientation and precipitates. Careful observation of specimen surfaces showed that, in many materials, micro-cracks are initiated from slip bands, which are formed in the very early stage of fatigue, and stretch across one grain^[3]. The initiation of fatigue crack along slip bands is known to be caused by irreversible plastic deformation in the localized slip bands under cyclic

Received: 2011-12-17

VRL: http://www.cnki.net/kcms/detail/11.2297.V.20121218.0859.201212.2778_021.html

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stress. The irreversible deformation and eventual crack initiation life was theoretically treated by Tanaka and Mura^[4]. For the case of one micro-crack initiation from a slip band, the method to solve this problem is often the Tanaka-Mura model:

$$N_c = \frac{8GW_s}{\pi(1-\nu)L(\Delta\tau-2k)^2} \quad (1)$$

where N_c is the micro-crack initiation cycle number, G is the shear modulus, W_s is the specific fracture energy per unit area, ν is the Poisson's ratio, L is the slip band length, $\Delta\tau$ is the average shear stress range on the slip band, and k is the frictional stress of dislocations on the slip plane. Equation (1) relates stress level at the initiation site and length of the slip band to the number of cycles to crack initiation. Hoshide and Kusuura^[5] applied this equation to simulate the fatigue behavior for a steel and two tapes of Titanium alloys under multi-axial loading. In that paper, crystal grains were simulated by deformed two-dimensional (2-D) hexagons and anisotropic stress-strain response was not taken into account. Brückner and HUANG^[6] applied this equation to simulate the fatigue crack initiation for a martensitic steel with a random grain structure. The elastic orthotropic material behavior was simulated preliminarily by 2-D element structures, and micro-crack coalescence was not considered. HUANG and Brückner, et al^[7] then studied a simplified three-dimensional model of the micro-structure to simulate the inhomogeneous stress distribution and its influence on multi-crack initiation behavior in a martensitic steel. Jezernik and Kramberger^[8-9] added three improvements to the model in Ref. [6] (multiple slip bands, micro-crack coalescence and segmented micro-crack generation), a macro-crack about 0.5 mm was finally formed, while the segmented micro-crack generation treatment is not reasonable. In Tanaka-Mura's model, equation (1) is deduced based on the theory that dislocation pile up along the slip band when the slip band impinges against the grain boundary, so L in equation (1) is the whole slip band length

across the grain. According to the experimental observation by Brückner^[6], the average size of the one segment cracks (i. e. the micro-cracks with no kinks) is somewhat correspond to grain size. So the segmented slip band assumption in a grain is debatable.

This article presents a microstructure-based fatigue-crack-initiation numerical model whose aim was to simulate the micro-crack initiation, growth and coalesce process in a Ni-base PM alloy (FGH 96) structure. In this model, the orthotropic effect to the inhomogeneous stress distribution in different grains and its influence on the multi-crack initiation behavior is obtained. Fatigue-crack-initiation models proposed by Tanaka and Mura for treating fatigue-crack initiation at slipbands, inclusions and notches are incorporated into the simulation model.

1 Theoretical models for fatigue crack initiation

Recent fatigue-crack-initiation models incorporate microstructure parameters in a direct and explicit manner. In a series of articles, Chan, Tanaka and Mura^[1,4,10] have advanced dislocation models for treating fatigue-crack initiation at slipbands, inclusions, and notches.

Tanaka and Mura proposed that systematic accumulation of dislocation dipoles within the localized slip bands and the resulting energy upon a critical value will lead to crack initiation. For crack initiation along a slipband, the crack initiation model in a grain can be obtained from equation (1). Similarly, the criterion for crack initiation by inclusion fracture due to impinging slip and dislocation pileup is given by

$$N_c = \frac{4G(G+G')W'_s}{\pi(1-\nu)G'L'(\Delta\tau-2k)^2} \quad (2)$$

Where G' is the shear modulus of the inclusion, L' is the inclusion size, W'_s is the specific fracture energy per unit area of inclusion. Another model applied to crack initiation from notches was proposed later. A new dislocation method was presented to evaluate the strain energy change due to a notch under load. Based on this model, a

notch with vanishing tip radius can be equivalent to a crack. Thus, one can calculate the fatigue crack initiation life initiated from another crack tip, as follows:

$$A = G/[2\pi(1-\nu)] \quad (3)$$

$$\Delta\gamma^n = \Delta\tau a^2/2A \quad (4)$$

$$c = a + L \quad (5)$$

$$\beta = 1 - (4k/\pi\Delta\tau)\arccos(a/c) \quad (6)$$

$$\Delta\gamma^l = (\beta\Delta\tau/\pi A)[c^2\arccos(a/c) - a(c^2 - a^2)^{1/2}] + (4ka/\pi^2 a) \times [(c^2 - a^2)^{1/2}\arccos(a/c) + 2a\ln(a/c)] \quad (7)$$

$$\Delta\gamma^t = (\beta\Delta\tau/2A)c^2 + (2ka/\pi A)(c^2 - a^2)^{1/2} \quad (8)$$

$$\Delta U_s = \Delta\tau(\Delta\gamma^t - \Delta\gamma^n)/2 - k\Delta\gamma^l \quad (9)$$

In equation (3)—equation (9), A and β are two intermediate scatters, a is the previous crack length in direction of the slip band that will initiate, c is the summation of a and L , $\Delta\gamma^n$ is the relative displacements due to the notch (crack), $\Delta\gamma^l$ is the relative displacements due to the slip band, $\Delta\gamma^t$ is the total relative displacements, ΔU_s is the increment of strain energy at each reversal of loading direction.

After N cycles of loading, the sum of the strain energy due to the dislocations accumulated along slip band is $2N\Delta U_s$. Based on the energy criterion, the stress cycles up to fatigue crack initiation N_c is expressed as

$$2N_c\Delta U_s = 4LW_s \quad (10)$$

Equation (1), equation (2) and equation (3)—equation (10), present the theoretical models for treating fatigue crack initiation from slip-bands, inclusions, and crack tips, respectively.

2 Numerical simulation models for fatigue-crack-initiation

2.1 Representative volume element

A representative volume element (RVE) is generated by the Voronoi's tessellation process, which simulates a small piece of material taken from the throat surface of a turbine disk specimen, as shown in Fig.1. A random orientation is assigned to each grain which represents the orientation of the crystallographic axes. Each cell

represents an alloy grain with specific crystal lattice orientation. This guarantees the material character of each grain is anisotropic, and the whole structure's behavior is isotropic. A three-dimensional RVE structure representing FCC polycrystals is shown in Fig.1. The arrow in each grain indicates the $[100]$ direction of the crystal lattice. The $[010]$ and $[001]$ directions are perpendicular to $[100]$ direction obeying the right hand rule.

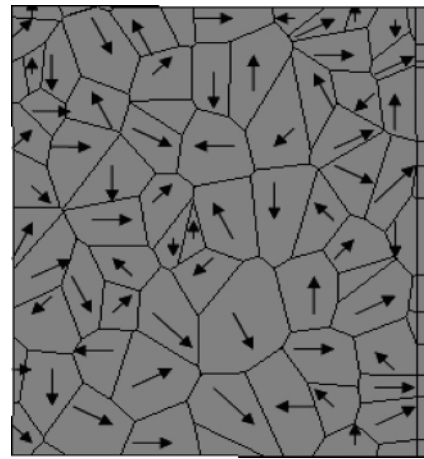


Fig.1 Three-dimensional representative element of polycrystalline structure

According to microcrystallography, octahedral $\{111\}$ planes are the highest atomic density planes which have the lowest slip resistance in FCC crystals. In the present simulation, the 12 possible slip systems are $[\bar{1}\bar{1}0] [\bar{1}01] [0\bar{1}1]$ in (111) plane, $[1\bar{1}0] [101] [011]$ in $(\bar{1}\bar{1}1)$ plane, $[110] [\bar{1}01] [011]$ in $(\bar{1}\bar{1}1)$ plane, and $[110] [101] [0\bar{1}1]$ in $(\bar{1}11)$ plane. For each grain, the slip system with maximum shear stress will be activated once the shear stress exceeds the frictional stress of dislocation.

A three-dimensional RVE structure has to take into account the random cell structure in space, their interaction with the adjacent grains, potential cracks which are not perpendicular to the surface, the 3-D orientation of the grains, and the 3-D stress state.

2.2 Coordinate systems

To deal with the random crystallographic orientation in pre-processing and post-process-

ing, three types of local coordinate systems are defined. For the first type, the axes of this local coordinate system coincide with the cubic lattice axes 123 of the grain as shown in Fig. 2(a) — Fig. 2(d). The orientations of coordinate axes x_i , y_i , z_i is determined (Fig. 2(a)) by three rotation angles from global coordinate system XYZ obtained by a random number generator. The orthotropic material characteristic is defined in this coordinate system. Fig. 2(b) indicates possible slip plane and orientations for the crack with respect to the lattice. The lattice is aligned with the system of coordinates, so the three axes x_i , y_i , z_i correspond to the $[100]$, $[010]$ and $[001]$ directions.

The second type of coordinate system is defined to identify the four slip planes for each grain. The slip planes are oblique to XY plane in the global coordinate system. For example (Fig. 2(c)), the coordinate system is generated by rotating 35.26° around $[1\bar{1}0]$ direction of (110) plane to represent the slip plane (111) . However, they are simulated as the true orientation in the post-processing of finite element analysis and presumed to be perpendicular to the XY -plane in the crack construction process to simplify the simulation model.

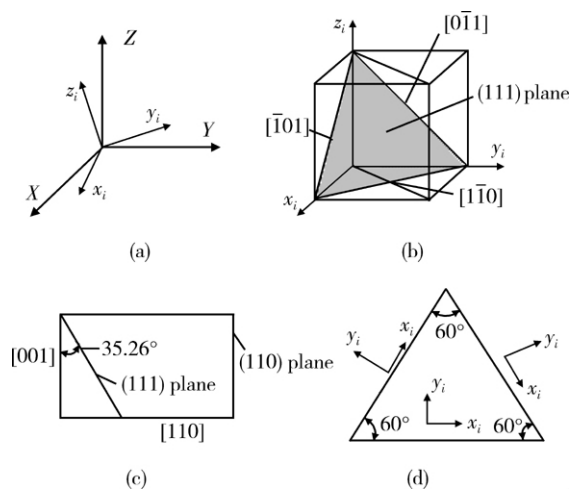


Fig. 2 Definition of local coordinate systems in 3-D mode

The third type of local coordinate system is defined to obtain the shear stress $\Delta\tau$ in slip directions for each slip plane. For the direction

$[1\bar{1}0]$, $[\bar{1}01]$, $[0\bar{1}1]$ in (111) plane, the coordinate system is generated by rotating 60° around z_i axis of the second type of coordinate system that represent the slip plane (110) .

2.3 Physical modelling

The crack initiation problem is studied on the throat surface of a Ni-base powder metallurgy specimen. Through stress analysis of the disk specimen, one can see that the maximum stress point (red area in Fig. 3) is in the throat surface. In the fatigue test, fatigue crack initiated from this critical area and eventually lead to the specimen failure. The fatigue-crack-initiation simulation model is shown in Fig. 4. The global model in Fig. 4 represents throat part of the specimen subjected to a given load level. The sub-model in Fig. 4 is a small local portion on the edge of the throat where the highest stresses are present and the formation of cracks is expected. The size of sub-model has been chosen $R = 0.38\text{ mm}$ from the critical point, which is prescribed in the damage tolerance design engineering. The sub-model contains a layer of grains, of which the

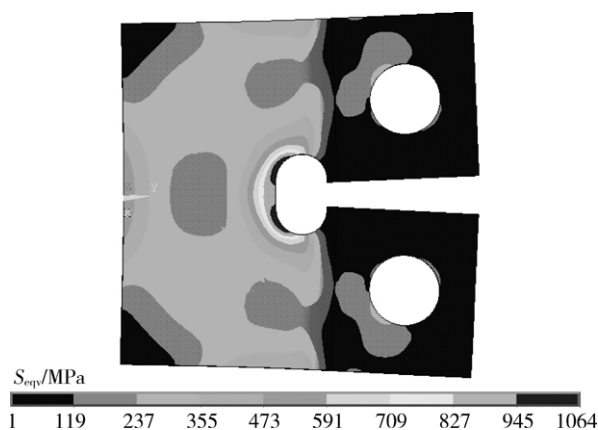


Fig. 3 Von Mises equivalent stress distribution of the specimen

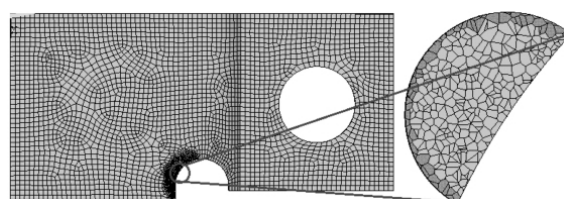


Fig. 4 Fatigue-crack-initiation simulation 1/2 model

thickness is $20\ \mu\text{m}$. Loading of a sub-model is implemented by applying stress distribution along the boundaries of the sub-model in global model.

A series of microstructures with various precipitate size distributions and volume fractions obtained by different thermo-mechanical processing are considered. The corresponding parameters of the constitutive model in Table 1 are obtained for IN100^[2]. A typical microstructure for Ni-base superalloy Udimet 720 Li, of which the microstructure is the same as FGH96, is shown in Fig. 5.

Table 1 Components of material IN100 constitutive matrix

	C_{11}/MPa	C_{12}/MPa	C_{44}/MPa
Matrix	158 860	73 910	130 150
Precipitate	135 000	59 210	81 515

Note: C_{11} , C_{12} , C_{44} are corresponding items of grain constitutive equation matrix IN 100.

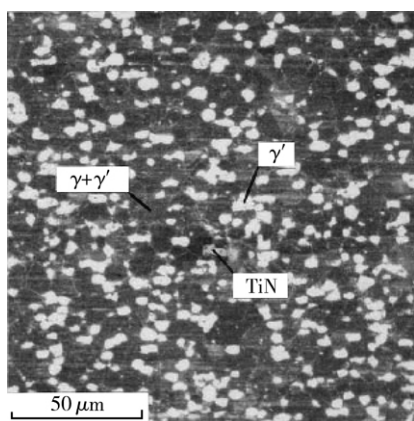


Fig. 5 Microstructure for Ni-base superalloy Udimet 720 Li with large γ' precipitates^[11]

Each grain of the sub-model is assigned to a random orientation, so each grain is anisotropic and the whole model is isotropic. The material parameters of the matrix and precipitate are defined in such a way that the original random orientation vector corresponds to the $[100]$, $[010]$ and $[001]$ direction in each element set. Considering the average grain size of $20\ \mu\text{m}$ the whole model consists of approximately 350 individual grains. The surrounding grains (in green area of

sub-model in Fig. 4) have to be excluded in micro-crack evaluation for the stress mismatch on sub-model boundary elements.

The stress distribution in the random grain structure with or without cracks is calculated. Fig. 6 shows the local shear stress distribution with no cracks.

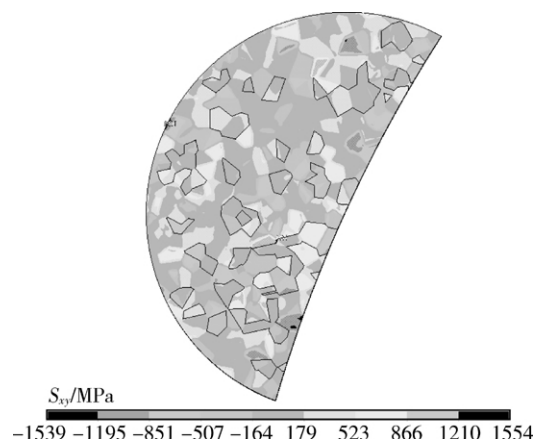


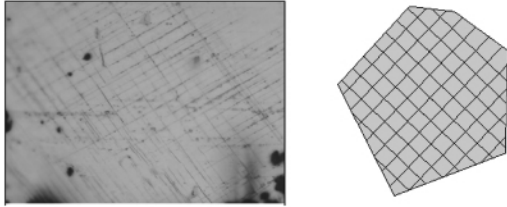
Fig. 6 Shear stress distribution of grains

The shear stress varies slightly within each grain, and varies from grain to grain especially for grains from different phases as a result of different crystal lattice orientations and the $\gamma-\gamma'$ mismatch. The grains with high values of the resolved shear stress are the ones in which micro-cracks will be formed in the early stages of the fatigue.

2.4 Definition of cracking path

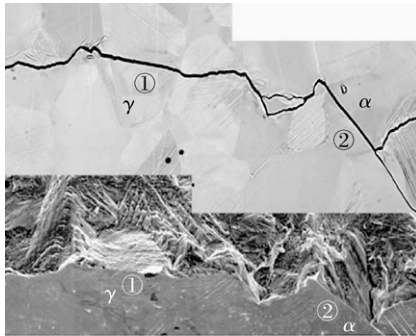
When simulating a micro-crack initiating along a slip band, the slip system should be defined. For each grain, there are four octahedral slip planes created through the centre of the grain, and additional slip planes are created with a $2\ \mu\text{m}$ offset from the previous slip plane. One of these slip planes will be the first to nucleate under fatigue loading. Fig. 7 shows slip bands of a Ni-base superalloy MAR-M-002 crystal, which has the same slip system as a FGH 96 crystal. For the grain where the neighboring grain already cracked, the initiation site is at the intersection of crack and grain boundary as a result of stress concentration around the crack tip. A new crack will then initiate along a slip plane near the initiate site. Fig. 8(a) shows the experimen-

tal observed picture of a trans-granular crack propagates across steel grains. Fig. 8(b) shows the sketch map of numerical simulation models. The slip planes (111) (−1−11) (1−11) and (−111) in Fig. 8(b) are the potential crack initiation paths.

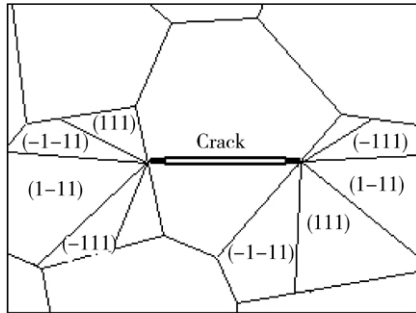


(a) Experiment observed picture^[12] (b) Sketch map of simulation model

Fig. 7 Crystal grain with multiple slip bands



(a) Experiment observed picture^[13]



(b) Sketch map of simulation model

Fig. 8 Transgranular crack-initiation across grains

2.5 Crack initiation life

Finite element analysis yields the stress field at the nodal points of the mesh. The value of resolved shear stress is calculated from the average shear stress, which can be derived from shear stress on the slip orientation along slip bands.

$$\tau^1 = \frac{1}{S} \sum_{i=1}^m \left(\frac{\tau_{i1}^1 + \tau_{i2}^1 + \tau_{i3}^1 + \tau_{i4}^1}{4} \right) \Delta S_i \quad (11)$$

$$\tau^2 = \frac{1}{S} \sum_{i=1}^m \left(\frac{\tau_{i1}^2 + \tau_{i2}^2 + \tau_{i3}^2 + \tau_{i4}^2}{4} \right) \Delta S_i \quad (12)$$

$$\Delta \tau = \tau^1 - \tau^2 \quad (13)$$

Here, τ^1 (τ^2) is the average shear stress along the slip band under uploading (unloading). $\Delta \tau$ is the range of resolved average shear stress. τ_{i1}^1 , τ_{i2}^1 , τ_{i3}^1 , τ_{i4}^1 (τ_{i1}^2 , τ_{i2}^2 , τ_{i3}^2 , τ_{i4}^2) are the resolved nodal shear stress of element i under uploading (unloading), where i is an index for counting the element, and m is the number of elements in the slip plane. ΔS_i is the area of the slip plane in element i , and S is the area of the slip plane in a grain.

Since the proposed algorithm for crack initiation goes through multiple iterations, it is necessary to keep track of the damage accumulation for every slip band over previous stages. In the beginning, total deformation energy needed for micro-crack initiation is calculated for every slip band of every grain, using equation (14)

$$U_s^{\text{th}} = 4W_s L \quad (14)$$

Then, the amount of deformation energy ΔU_s generated per cycle for every slip band is calculated. If an isolated micro-crack initiated from a slip band,

$$\Delta U_s = \frac{\pi(1-\nu)(\Delta \tau - 2k)^2 L^2}{2G} \quad (15)$$

If a micro-crack is initiated from the tip of previous crack, then ΔU_s is calculated by following equation (3)–equation (10).

The number of loading cycles N_s^j , required for a micro-crack nucleation on stage j for each slip band, is calculated with the following equation:

$$N_s^j = (U_s^{\text{th}} - U_s^{j-1}) / \Delta U_s \quad (16)$$

where U_s^{j-1} represents the already accumulated damage in each slip band at the stage $j-1$. The smallest number $N_{s,\min}^j$ of all slip bands is the micro-crack initiation number at stage j . For other slip bands, the accumulated damage U_s^j for stage j is

$$U_s^j = U_s^{j-1} + \Delta U_s N_{s,\min}^j \quad (17)$$

The sum of $N_{s,\min}^j$ for all stages represents the total crack initiation life N

$$N = \sum_{j=1}^n N_{s,\min}^j \quad (18)$$

3 Numerical simulation and experimental results

Numerical simulation was performed on the finite element model, using a plug-in that was written in ANSYS parametric design language (APDL) specially for handling micro-crack nucleation and growth. Fig.9 (a)—Fig.9 (d) show a few stages of micro-cracks evolution. It can be seen that the first micro-crack nucleate in a grain near the surface. Then, the micro-crack propagation is blocked by a precipitate. In the meantime, another micro-crack nucleates in a large grain and gradually propagate into a larger micro-crack perpendicular to the first principal stress direction. When micro-cracks propagate through the whole model, a macro-crack is mainly formed, and the simulation is stopped.

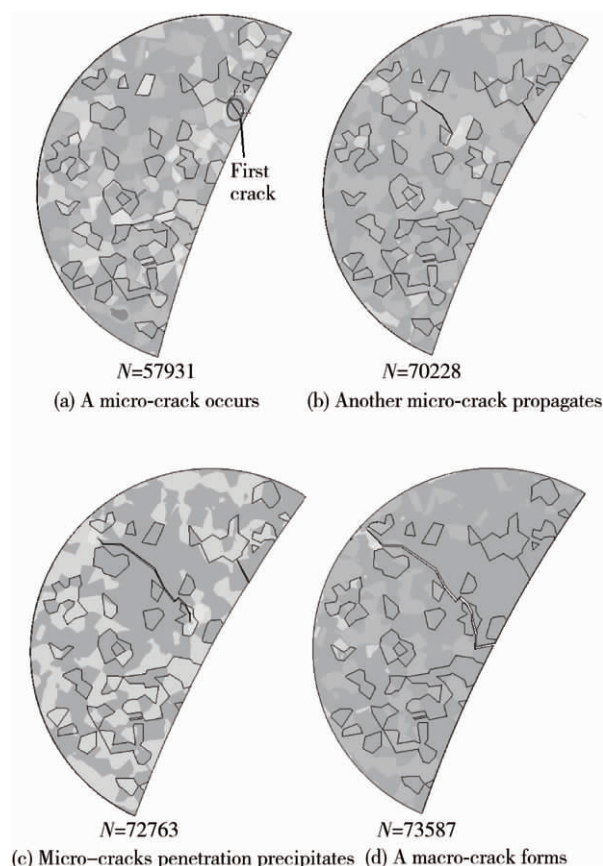


Fig. 9 Four stages of micro-cracks evolution

Fatigue tests have been carried out on a pulsating machine INSTRON-8802 with uniaxial loading and load control. The loading spectrum

is applied as triangular waves with constant amplitude. The stress ratio $R_s=0.04$, and the upload is 6090 N, download is 270 N. The used frequency of loading is approximately 2 Hz and testing temperature is 580 °C. Five specimens have been loaded at the same stress level. The structure and size of specimens is shown in Fig.10.

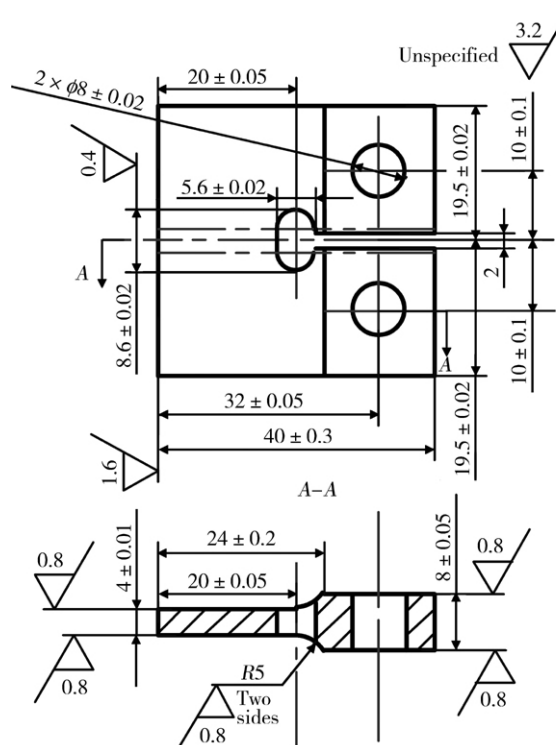


Fig. 10 Structure and size of the specimen (unit: mm)

All the five crack initiation points are adjacent to the tangent point of raceway-shaped holes and a little deflected to the arc section. The picture of a cracked specimen is shown in Fig.11. The experimental results of low cycle fatigue crack-initiation life are shown in Table 2.



Fig. 11 Picture of a cracked specimen

Table 2 Experimental LCF crack-initiation life of specimens

Specimen number	Upload/ N	Download/ N	Frequency/ Hz	Life/ cycle
1	6 090	270	2	69 000
2	6 090	270	2	90 000
3	6 090	270	2	41 000
4	6 090	270	2	93 000
5	6 090	270	2	81 000
The average life				74 800

The average experiment life is 74800 cycles. The fatigue initiation life simulated is 73587 cycles, which is consistent well with the experimental result.

4 Conclusions

The present paper has applied material parameters and microstructure features of the PM alloy to the simulation of fatigue crack initiation. A 3-D numerical simulation of the fatigue crack initiation on a turbine disk specimen was implemented for the first time. Four improvements were made in the simulation:

1) Considering of crack initiation along 12 principal slip systems on $\{111\}$ octahedral slip planes of FCC crystal in 3-D models.

2) Considering influence of coherent γ' precipitate due to impinging slip and dislocation pileup.

3) The Tanaka-Mura theory of the fatigue crack initiation from notches is applied to simulate the crack initiate from another crack tip.

4) The coalescence of random initiated micro-cracks is simulated once they intersect with each other and a macro-crack is finally formed.

It is shown that the simulation has a reasonable correlation with experimental testing, but it still has some deficiencies. All the cracks are presumed to be trans-granular cracks that are accumulated along slip bands, the inter-granular cracks are not taken into account. Otherwise, the number of loading cycles needed for a crack to stride over grain boundaries is not considered. Further investigation need to be conducted in the

future work.

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