The Reliability of the Finite Element Simulation of the Interface Mechanical Effect of Inclusion and Matrix Material in Powder Metallurgy Superalloy

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Abstract. The inclusion defects in powder metallurgy superalloy have the characteristics of randomness, such as the shape, size, location and composition. It is important to establish effective and reliable finite element model and method to study the influence of the different defects. In this paper, the inclusion/matrix interface model was proposed, and on the basic theory of two-dimensional elastic problems of complex variable function, the analytical formula was derived and the analytical solution was calculated for the condition of circular inclusion in matrix. On the other hand, stress distribution of the interface of inclusion and matrix was simulated by finite element method. The finite element model is proved effective, reliable through comparison analysis between the numerical analysis method and finite element simulation.

1. Introduction

Due to the manufacturing process characteristics of powder metallurgy superalloy, the defects are inevitable. At present, inclusion is the main defect category in powder metallurgy superalloy. The inclusion can reduce the fatigue performance, especially the low cycle fatigue property of powder metallurgy superalloy. Different from common particle, fiber reinforced composite materials, inclusions in powder metallurgy superalloy have characteristics of random in aspects of shape, size, location and composition, and cannot establish the overall model using macro homogenization method. Therefore, it is of great significance to study the mechanical effect of inclusions in the matrix.

The main test methods to study the defects are low cycle fatigue tests and analysis from the fracture surfaces, and using statistical method to study the relationship between the test conditions and the defects. Although this method may give the relationship between defects and macroscopic mechanics, the defects influence cannot be studied fully because the randomness of the shape, size, location and composition of the defects. The computer simulation is an important aided method. The interface of defect and matrix improves the simulation complexity. Reliable simulation methods and models are the prerequisite for researching the defects.

Lin Tao \cite{1} analysed the effect of shot peening on powder metallurgy superalloy using ABAQUS software, established the finite element model of a single projectile impacting target material, compared the residual stress and equivalent plastic strain of different velocity and surface friction factor, the collision frequency and the distance of projectiles. A numerical simulation of the isothermal forming process of precasting plate of powder metallurgy superalloy was carried out \cite{2, 3}. The
heating process of isothermal forging mould of FGH96 superalloy plate was simulated with FEA by Zhang Mingjie et al. [4]. The stress field and temperature field of the mould during the heating process were studied, the thermal damage caused by thermal fatigue was analysed, and the heating system of the mould was optimized. It is lacking on interface stress analysis of powder metallurgy superalloy by FEA.

The inclusion/matrix interface is a weak joint surface, easy to cause crack initiation and fracture damage, and the mechanical effect produced by inclusion in the matrix is determined by the interface stress distribution of inclusion and matrix. In order to study the reliability of finite element simulation results, the distributions of stress and strain of inclusion interior, matrix nearby inclusion and the interface of inclusion/matrix were comparatively analysed by theoretical derivation and the analytical solution and numerical simulation method. On the other hand, the effect of finite size boundary conditions on the stress distribution was also considered, the validity and reliability of finite element model was studied in this article.

2. Research method

The matrix and inclusions are completely elastic material, where the elastic modulus of the matrix $E_1 = 193000$MPa, the Poisson's ratio $\nu_1 = 0.3$, the elastic modulus of $Al_2O_3 E_2 = 400000$MPa, and Poisson's ratio $\nu_2 = 0.3$.

![Diagram of interface connection model and interface phase](image)

Figure 1. Interface connection model and interface phase model diagram.

Using the inclusion/matrix two-phase model, the interface was considered as the geometric curve or surface of the bonded matrix with the inclusion phase, and the bond strength is certain. In this paper, the circular inclusion and the excellent interface was studied. The boundary conditions of the stress and displacement were as follows.

$$
\sigma_r^{(1)} = \sigma_r^{(2)}, \tau_{rr}^{(1)} = \tau_{rr}^{(2)}, u_1^{(1)} = u_2^{(2)}, v_1^{(1)} = v_2^{(2)}
$$

According to the boundary conditions of upper formula and the geometrical and physical relations of elastic mechanics, it can be seen that the normal strain and the shear strain perpendicular to the interface are discontinuous. The normal stress parallel to the interface is also discontinuous. Based on these considerations, the interfacial normal stress and the interface shear stress are main destruction parameters, and the maximum main stress and maximum plastic strain are main destruction parameters of matrix.

According to the basic theory of complex function, the stress components can be expressed separately [5].

$$
\begin{align*}
\sigma_x &= 2 \text{Re} \Phi(z) - \text{Re} [\overline{\Phi'}(z) + \Psi(z)] \\
\sigma_y &= 2 \text{Re} \Phi(z) + \text{Re} [\overline{\Phi'}(z) + \Psi(z)] \\
\tau_{xy} &= \text{Im} [\overline{\Phi'}(z) + \Psi(z)]
\end{align*}
$$

(1)

The function expression of the displacement component can be obtained according to the geometric equation and the physical equation of the elastic theory.
\[ 2\mu(u + iv) = \kappa \phi(z) - z\phi'(z) - \psi(z) \]  \hspace{1cm} (2)

\( U \) and \( v \) are the displacement of two directions in a rectangular coordinate system. \( \mu \) is the shear modulus, \( \mu = E / (2(1 + \nu)) \), \( E \) is modulus of elasticity, \( \nu \) is Poisson's ratio. \( K \) is the combination parameter of the material, and \( \kappa = (3 - \nu) / (1 + \nu) \) under plane stress condition, \( \kappa = 3 - 4\nu \) under plane strain condition.

In the infinite and multiply connected area, the stress function may be represented by the following two analytic functions.

\[
\begin{align*}
\phi(z) &= -\frac{F_x + iF_y}{2\pi(1 + \kappa)} \ln z + (B + iC)z + \phi_0(z) \\
\psi(z) &= \frac{\kappa(F_x - iF_y)}{2\pi(1 + \kappa)} \ln z + (B' + iC')z + \psi_0(z)
\end{align*}
\]  \hspace{1cm} (3)

\( F_x \) and \( F_y \) are the sum of all the external forces on the edge of the hole, \( B, B', C, C' \) are the combined expressions of the far field load, \( B = \frac{\sigma_{xy} + \sigma_{yx}}{4}, \ C = 0, \ B' = \frac{\sigma_{xy} - \sigma_{yx}}{2}, \ C' = \tau_{xy}, \ \psi_0(z) \) and \( \psi_0(z) \) are just the items of negative power of \( z \).

3. Analytic solution of the stress distribution of circular inclusions in the matrix

The complex function elastic theory was used to obtain the analytic formula. Based on the analytic calculation formula, the interface stress of circular inclusion of infinite flat bearing two-way tensile load was calculated.

3.1. Mechanical model

As shown in figure 2 (a), infinite flat is subjected to a two-way tensile load in the \( y \) direction at infinity. A circular inclusion with radius \( R \) is in the center of the plate, the plate’s material constants are \( \mu_1 \) and \( \kappa_1 \), the inclusion’s material constants are \( \mu_2 \) and \( \kappa_2 \). The matrix and inclusion is perfectly connected and the interface is the boundary between the two different materials. The interface model and its boundary conditions are shown in figure 2 (b). (Note: mark 1 refers to matrix, 2 refers to inclusions)

![Inclusion in the plate and diagrammatic sketch of angle θ](image)

\( \text{Figure 2. Inclusion and diagrammatic sketch of angle } \theta \)
corresponding region. Then, it may be transformed into solving the problem of linear equations using interface and infinity boundary conditions. The last, according to the relationship between analytical function and stress, one-way tensile problem of a single circular inclusion is obtained.

Because the interfacial boundary of inclusion and matrix is arc, boundary conditions of the interface are not easy to represent in rectangular coordinates, then it is need to be converted to polar coordinates. It can be seen from the geometric knowledge that the displacement \((u, v)\) in the polar coordinates and the displacement in the rectangular coordinate system have the following coordinate changes.

\[
\begin{align*}
    u_r &= u \cos \theta + v \sin \theta \\
    u_\theta &= -u \sin \theta + v \cos \theta
\end{align*}
\]  

(4)

Complex function \(u_r + i u_\theta\) is composed of the upper form:

\[
u_r + i u_\theta = (u + iv)e^{-i\theta}
\]

(5)

Complex expression of the displacement of the rectangular coordinate system is substituted into the formula (2), which is the complex representation of the polar coordinates.

\[
2\mu(u_r + i u_\theta) = e^{-i\theta}\left[k\phi(z) - z\phi'(z) - \psi(z)\right]
\]

(6)

As shown in figure 3, it is necessary to establish the stress equilibrium condition of the interface microelement in order to obtain the normal stress and shear stress of the inclusion and matrix interface of the polar coordinates. The surface area of the microelement cant is \(dA\), the circle angle is \(\theta\), and the micro-equilibrium equation in both X and Y directions are as follows.

\[
\begin{align*}
    \sigma_{rr} \cdot dA \cdot \cos \theta + \tau_{r\theta} \cdot dA \cdot \sin \theta - \tau_{x\theta} \cdot dA \cdot \sin \theta - \sigma_{x\theta} \cdot dA \cdot \cos \theta &= 0 \\
    \sigma_{rr} \cdot dA \cdot \sin \theta - \tau_{x\theta} \cdot dA \cdot \cos \theta - \tau_{r\theta} \cdot dA \cdot \cos \theta - \sigma_{x\theta} \cdot dA \cdot \sin \theta &= 0
\end{align*}
\]

(7)

Remove \(dA\), according to the square formula of the trigonometric functions we can obtain the function as follows.

\[
\begin{align*}
    \sigma_{rr} &= \frac{1}{2}(\sigma_r + \sigma_s) + \frac{1}{2}(\sigma_r - \sigma_s) \cos 2\theta + \tau_{x\theta} \sin 2\theta \\
    \tau_{r\theta} &= \frac{1}{2}(\sigma_r - \sigma_s) \sin 2\theta + \tau_{x\theta} \cos 2\theta
\end{align*}
\]

(8)

Notice that negative values of \(\sigma_{rr}, \tau_{r\theta}\) represent the opposite direction.

![Figure 3](image)

**Figure 3.** A schematic diagram of the force of the microelement near the interface.

Combine equation (8) with equation (1),
\[
\sigma_{rr} - i\sigma_{r\theta} = \varphi'(z) + \overline{\varphi'(z)} - e^{i\varphi(z)} + \psi'(z)
\]
(9)

Through the above analysis, we have a complex expression of displacement and stress in polar coordinates.

\[
\left\{ \begin{array}{l}
2\mu(u + iv) = e^{-i\theta} \left[ \kappa \varphi(z) - z\varphi'(z) - \psi(z) \right] \\
\sigma_{rr} - i\sigma_{r\theta} = \varphi'(z) + \overline{\varphi'(z)} - e^{i\varphi(z)} + \psi'(z)
\end{array} \right.
\]
(10)

Substitute the far load conditions \(\sigma_x^\infty = 0, \sigma_y^\infty = P, \tau_{xy}^\infty = 0\) into the formula (3), then the infinite plane area with round hole can be expressed as:

\[
\varphi_1(z) = \sum_{n=1}^{\infty} a_n \left( \frac{R}{z} \right)^n + \frac{P}{4} z
\]
(11)

\[
\psi_1(z) = \sum_{n=1}^{\infty} b_n \left( \frac{R}{z} \right)^n + \frac{P}{2} z
\]

According to the series theory in the complex function, the complex expression of the circular area domain is obtained.

\[
\varphi_2(z) = \sum_{n=1}^{\infty} c_n \left( \frac{z}{R} \right)^n
\]
(12)

\[
\psi_2(z) = \sum_{n=1}^{\infty} d_n \left( \frac{z}{R} \right)^n
\]

According to the displacement continuity conditions of the interface, we may obtain:

\[
\varphi_1(z) = \frac{P}{2} \left( \frac{\mu_2 - \mu_1}{\mu_2 \kappa_1 + \mu_1} \right) R^2 z + \frac{P}{4} z
\]
(13)

\[
\varphi_2(z) = \frac{P}{2} \left( \frac{\kappa_1 - \mu_1 \kappa_2 + \mu_1 - \mu_2}{2 \mu_2 + \mu_1 \kappa_2 - \mu_1} \right) R^2 z
\]

\[
+ \frac{P}{2} \left( \frac{\mu_1}{\mu_2 \kappa_1 + \mu_1} \right) R^4 z^3 + \frac{P}{2} z
\]

\[
\psi_1(z) = \frac{P}{2} \left( \frac{\mu_2 (\kappa_1 + 1)}{4 (\kappa_2 - 1) \mu_1 + 2 \mu_2} \right) z
\]
(14)

\[
\psi_2(z) = \frac{P}{2} \left( \frac{1 + \kappa_1}{\mu_1 + \mu_2 \kappa_1} \right) z
\]

Substitute the formula (14) into formula (1), then the stress components in the rectangular coordinate system can be obtained.
Substitute the formula (15) into formula (9), then the stress component in polar coordinates can be obtained.

\[
\begin{align*}
\sigma^{(2)}_{rr} &= \frac{P}{2} \frac{\mu_2 (\kappa_1 + 1)}{(\kappa_2 - 1) \mu_1 + 2 \mu_2} - \frac{P}{2} \frac{\mu_2 (1+\kappa_1)}{\mu_1 + \mu_2 \kappa_1} \\
\sigma^{(2)}_{x\theta} &= \frac{P}{2} \frac{\mu_2 (1+\kappa_1)}{(\kappa_2 - 1) \mu_1 + 2 \mu_2} + \frac{P}{2} \frac{\mu_2 (1+\kappa_1)}{\mu_1 + \mu_2 \kappa_1} \\
\tau^{(2)}_{x\theta} &= \frac{P}{2} \frac{\mu_2 (1+\kappa_1)}{\mu_1 + \mu_2 \kappa_1} \sin 2\theta
\end{align*}
\]

(15)

Substitute the material parameters under the condition of plane stress \(\mu = E/2(1+\nu)\), \(\kappa = (3-\nu)/(1+\nu)\) and material parameters under the condition of plane strain \(\mu = E/2(1+\nu)\), \(\kappa = 3 - 4\nu\) into formula (15), then under the condition of plane stress,

\[
\begin{align*}
\sigma^{(2)}_{rr} &= \frac{P}{E_1} \frac{1}{1+\nu_v} + \frac{1}{E_2} \frac{2 \cos 2\theta}{E_1 + E_2} \\
\sigma^{(2)}_{x\theta} &= \frac{2PE_v \sin 2\theta}{E_1(1+\nu_v) + E_2(3-\nu_v)} \\
\tau^{(2)}_{x\theta} &= \frac{2PE_v (1-\nu_v)(1+\nu_v)}{E_1(1+\nu_v) + E_2(3-4\nu_v)} \sin 2\theta
\end{align*}
\]

(16)

(17)

Under the condition of plane strain,

\[
\begin{align*}
\sigma^{(2)}_{rr} &= \frac{P(1-\nu_v)}{E_1} \left[ \frac{1}{(1-2\nu_v)(1+\nu_v)} + \frac{1}{E_v} \frac{2 \cos 2\theta}{E_1(1+\nu_v) + 3-4\nu_v} \right] \\
\sigma^{(2)}_{x\theta} &= \frac{2PE_v (1-\nu_v)(1-\nu_v)}{E_1(1+\nu_v) + E_2(1+\nu_v)(3-4\nu_v)} \sin 2\theta
\end{align*}
\]

(18)

3.3. Analytical calculation and result analysis

From equation (15), we know that the stress components of the circular inclusion in rectangular coordinate systems, \(\sigma_x, \sigma_y, \tau_{xy}\) are independent of the coordinates, and they are constant parameters related to material and load conditions.

The stress components of the interface of the matrix/inclusion are material correlation. The matrix material is FGH95 powder metallurgy superalloy, and the modulus of elasticity E is 193000MPa, poisson’s ratio is 0.3. The inclusion is Al_2O_3, and the modulus of elasticity E is 400000Mpa, poisson’s ratio is 0.3. The load is 100Mpa. All of the parameters are substituted into equation (17) and (18), the relationships between interface stress and angle \(\theta\) under plane stress and plane strain, as shown in figure 4.
Figure 4. The stress component of the interface varies with angle θ.

It can be seen from figure 4 that the interface stress components have the same trend as the circumferential angle θ under the plane stress condition and the plane strain condition. At the same circumferential angle θ, the interfacial stress component under the plane stress condition is higher than that under the plane strain condition. In addition, from the trend of each curve, the interface normal stress reaches the maximum at the 90° circumference angle θ, and the interface shear stress reaches the maximum at θ 45° and 135°. The interface normal stress and the interface shear stress are the main stress components to measure the interfacial strength. Considering the law of the interface normal stress and shear stress in the range of 0~180°, we consider that the interface area of 45~135° is dangerous.

4. Finite element simulation of stress distribution of circular inclusion in matrix

Using the finite element software Abaqus, the two-dimensional plane problem with circular inclusion in the case of uniaxial stretching is simulated. The reliability of the finite element model is verified by comparing the numerical solution with the analytical solution.

4.1. Finite element model

For simulating the far-off boundary conditions, the inclusion size and the finite large plane size proportion is set to 1 to 10000. The matrix size is 1 m long and 1 m width. The radius R of inclusion is 100 um (equivalent to the size of inclusion in powder metallurgy superalloy). Taking into account the symmetry of the load and geometry, a quarter of the whole was used to build the model.

4.2. Grid division

Considering the difference between the size of inclusion and the size of the matrix, the grids are divided in a hierarchical manner. In addition, in order to obtain the stress value conveniently and accurately at different angle θ, the grid seeds of the interface of the inclusion/matrix are divided into 48 parts within the scope of 0~90°. The angle span of every four grid nodes is 7.5°.

4.3. Results analysis of finite element simulation

Stress component distributions inside of the inclusion under the conditions Plane stress and plane strain are shown in figure 5 and figure 6. S11, S22, S33 represent the stress of the X direction, Y direction and Z direction of the unit cell of the normal stress, and the positive symbol is tensile stress, the negative symbol is pressure stress. The S12 is the shear stress of the unit cell along the Y axis, and the clockwise sign is positive, the counter clockwise sign is negative.
You can see from the figure 5, 6 that each stress component inside of the inclusions is constant under rectangular coordinate system whether it is plane stress or plane strain condition, which is consistent with the result of the analytic solution.

![Stress component distributions inside of the inclusion under the conditions Plane stress.](image)

**Figure 5.** Stress component distributions inside of the inclusion under the conditions Plane stress.

![Stress component distributions inside of the inclusion under the conditions Plane strain.](image)

**Figure 6.** Stress component distributions inside of the inclusion under the conditions Plane strain.

Through formula (9), stress component under rectangular coordinate system can be transferred to normal stress and shear stress of the interface, the calculation results after the transformation are shown in table 1, 2. The analytical solution and the finite element results were compared in figure 7, from figure 7, the finite element calculation result is consistent with the analytic solution, which shows that the finite element calculation model is reliable.
Table 1. Interface stress under the conditions Plane stress.

| $\theta$ (°) | $\sigma_{rr}$ (MPa) | $\tau_{r\theta}$ (MPa) | $\theta$ (°) | $\sigma_{rr}$ (MPa) | $\tau_{r\theta}$ (MPa) |
|--------------|---------------------|------------------------|--------------|---------------------|------------------------|
| 0.000        | 0.948               | 0.000                  | 52.500       | 76.617              | 58.062                 |
| 7.500        | 2.996               | 15.558                 | 60.000       | 91.115              | 52.057                 |
| 15.000       | 9.001               | 30.055                 | 67.500       | 103.564             | 42.504                 |
| 22.500       | 18.554              | 42.505                 | 75.000       | 113.117             | 30.055                 |
| 30.000       | 31.003              | 52.057                 | 82.500       | 119.122             | 15.557                 |
| 37.500       | 45.501              | 58.062                 | 90.000       | 121.170             | 0.000                  |
| 45.000       | 61.059              | 60.111                 |             |                     |                        |

Table 2. Interface stress under the conditions Plane strain.

| $\theta$ (°) | $\sigma_{rr}$ (MPa) | $\tau_{r\theta}$ (MPa) | $\theta$ (°) | $\sigma_{rr}$ (MPa) | $\tau_{r\theta}$ (MPa) |
|--------------|---------------------|------------------------|--------------|---------------------|------------------------|
| 0.000        | -2.661              | 0.000                  | 52.500       | 74.551              | 59.247                 |
| 7.500        | -0.571              | 15.875                 | 60.000       | 89.344              | 53.119                 |
| 15.000       | 5.555               | 30.669                 | 67.500       | 102.048             | 43.372                 |
| 22.500       | 15.303              | 43.372                 | 75.000       | 111.795             | 30.668                 |
| 30.000       | 28.006              | 53.120                 | 82.500       | 117.923             | 15.875                 |
| 37.500       | 42.800              | 59.247                 | 90.000       | 120.013             | 0.000                  |
| 45.000       | 58.675              | 61.337                 |             |                     |                        |

Figure 7. The comparison of analytical solution and the finite element results.

5. Conclusions

(1) The necessary simplification is done for the interface of powder metallurgy superalloy and the inclusion, the interface from the mechanics meaning was defined, which is considered as the set curve or surface of the bonded matrix and the inclusion phase. Two phase model of inclusion and matrix interface in powder metallurgy superalloy is established.

(2) On the basic theory of two-dimensional elastic problems of complex variable function, the analytical formula is derived and the analytical solution is calculated for the condition of circular inclusion in matrix.

(3) The stress and displacement boundary conditions were defined under the condition of good connection interface between the inclusion and matrix in the two phase model. On both sides of the interface, the normal stress perpendicular to the interface is equal, the shear stress parallel to the
interface is equal and interface displacement is continuous. The evaluation parameters of interface cracking are determined as the normal stress and shear stress, and the model of interface stress analysis under different conditions is established.

(4) The validity and reliability of the finite element model are verified through comparing the numerical analysis method and the finite element simulation results.

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