MICROMECHANICS INVESTIGATION OF DEFECTS IN SOLID MATERIALS

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SCHOOL OF MECHANICAL AND AEROSPACE ENGINEERING

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Abstract

Microdefects such as cracks, vacancies, voids and inclusions are often formed in materials during their manufacturing processes or under working conditions. These defects have significant influences on the mechanical and physical properties of components, especially those for aerospace, automotive and offshore engineering applications, and may eventually result in the damages and failures of these components. Therefore, it is of great importance to investigate the mechanics of materials with these microdefects for the minimization of potential damage and failure of the components.

Firstly, a semi-analytic solution is proposed to solve the elastic-plastic fracture behaviors of an infinite space with multiple cracks and inhomogeneous inclusions under the remote tensile stress in this thesis. Based on the Equivalent Inclusion Method, each inhomogeneous inclusion can be modeled as a homogenous inclusion with the initial eigenstrains plus unknown equivalent eigenstrains. The cracks are regarded as a distribution of edge dislocations with unknown densities based on the Distributed Dislocation Technique. By using a modified conjugate gradient method, all the unknown equivalent eigenstrains and dislocation densities are obtained iteratively. The fast Fourier transform and discrete convolution are adopted to improve the computational efficiency. According to the Dugdale model, the plastic zone sizes of cracks can be obtained by canceling the stress intensity factor due to the closure stress and that due to the applied external loading. The effect of the Young’s moduli and positions of inhomogeneous inclusions on the plastic zone sizes is investigated.

Secondly, two semi-analytic solutions for the elastic-plastic fracture behaviors of a half-space with cracks subjected to the prescribed loading and contact loading
are also developed in this thesis. For the inhomogeneous contact problem, the unknown contact area and pressure can be obtained iteratively when the surface displacement induced by the subsurface cracks and contact loading converges with a numerical algorithm. According to the modified Dugdale crack model, it is found that the plastic zone sizes of crack tips are significantly influenced by the yield strength of the matrix material, the crack depth, the original crack length, and the external loading.

Thirdly, the elastic-plastic behaviors of a film-substrate with inhomogeneous inclusions under contact loading are studied by modeling the coating material as an inhomogeneous inclusion with respect to the substrate. A plasticity loop and an incremental loading process are used to obtain the accumulative plastic strain iteratively. This model considers not only the interaction among the contact loading body, embedded inhomogeneous inclusions and film materials, but also the elastic-plastic behaviors of the film-substrate system.

Finally, the elastic-plastic behaviors of a half-space with inhomogeneous inclusions and cracks subjected to contact loading are studied. This model considers not only the horizontal cracks but also the vertical cracks. The plastic zones in the half-space can be determined based on the substrate stress distribution and the von Mises yield criterion.

The research work in this thesis not only provides knowledge of the damage behaviors of materials containing microdefects, but also is of guiding significance for the improvements of functionality and reliability of engineering components.
List of Publications


List of Publications
Acknowledgements

First, I would like to express my heartfelt gratitude and appreciation to my supervisor Prof. Zhou Kun for his tremendous guidance, support, patience and encouragement during my PhD study. This research would be impossible without his instructive advice and help. I have immensely benefitted from his strict training on both scientific thinking and academic writing. His rigorous and serious attitude towards scientific research has deeply impressed me. I have been so fortunate to have the opportunity to work with him.

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<tr>
<td>( a_0 )</td>
<td>Hertz contact radius</td>
</tr>
<tr>
<td>( C_{ijkl}, C_{ijkl}^e, C_{ijkl}^p )</td>
<td>Elastic moduli of the substrate, coating layer or inclusion</td>
</tr>
<tr>
<td>( c^\perp, d^\perp, c^\parallel, d^\parallel )</td>
<td>Coefficients to approximate the dislocation densities</td>
</tr>
<tr>
<td>( d )</td>
<td>Coating thickness</td>
</tr>
<tr>
<td>( E_1, E_c, E_s )</td>
<td>Young’s moduli of the inclusion, coating layer or substrate</td>
</tr>
<tr>
<td>( E_{1s}, E_2 )</td>
<td>Young’s moduli of the sphere or cylinder, and half-space</td>
</tr>
<tr>
<td>( E' )</td>
<td>Effective Young’s modulus</td>
</tr>
<tr>
<td>( E_t )</td>
<td>Tangential modulus</td>
</tr>
<tr>
<td>( E_{ij}^\perp, E_{ij}^\parallel, F_{ij}^\perp, F_{ij}^\parallel )</td>
<td>Influence coefficients related to the stresses caused by dislocations</td>
</tr>
<tr>
<td>( H^\perp, K^\perp, H^\parallel, K^\parallel )</td>
<td>Influence coefficients related to the displacements caused by dislocations</td>
</tr>
<tr>
<td>( G_{ij}^\perp, G_{ij}^\parallel )</td>
<td>Influence functions related to the stress caused by dislocations</td>
</tr>
<tr>
<td>( K_1, K_{II}, K_{III} )</td>
<td>Stress intensity factor of the crack in modes I, II or III</td>
</tr>
<tr>
<td>( K_{1p}, K_{IIp} )</td>
<td>Stress intensity factor of the crack in modes I and II due to the closure stresses</td>
</tr>
<tr>
<td>( N_x, N_y, N_z )</td>
<td>Number of grid points in x-, y- or z-axis</td>
</tr>
<tr>
<td>( P )</td>
<td>Surface pressure</td>
</tr>
<tr>
<td>( R )</td>
<td>Sphere or cylinder radius involved in a contact system</td>
</tr>
<tr>
<td>( S )</td>
<td>Deviatoric stress</td>
</tr>
<tr>
<td>( u )</td>
<td>Surface displacement</td>
</tr>
<tr>
<td>( W )</td>
<td>Normal loading</td>
</tr>
<tr>
<td>( p_0 )</td>
<td>Maximum Hertz pressure</td>
</tr>
<tr>
<td>( \alpha_0, \beta_0, \gamma_0 )</td>
<td>Element index in x-, y- or z-axis</td>
</tr>
<tr>
<td>( \sigma_{VM} )</td>
<td>The von Mises equivalent stress</td>
</tr>
<tr>
<td>( \sigma^0 )</td>
<td>Eigenstress induced by the initial eigenstrain</td>
</tr>
<tr>
<td>( \sigma^* )</td>
<td>Eigenstress induced by the equivalent eigenstrain</td>
</tr>
<tr>
<td>( \sigma^{**} )</td>
<td>Eigenstress induced by the equivalent plastic strain</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>----------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>$\sigma^c$</td>
<td>Stress caused by dislocations</td>
</tr>
<tr>
<td>$\sigma^p$</td>
<td>Stress caused by surface pressure</td>
</tr>
<tr>
<td>$\sigma_{ys}, \sigma_{yi}, \sigma_{yc}$</td>
<td>Yield strength of the substrate, inclusion or coating</td>
</tr>
<tr>
<td>$\epsilon^0$</td>
<td>Initial eigenstrain</td>
</tr>
<tr>
<td>$\epsilon^*$</td>
<td>Equivalent eigenstrain</td>
</tr>
<tr>
<td>$\epsilon^{**}$</td>
<td>Equivalent plastic strain</td>
</tr>
<tr>
<td>$\nu_s, \nu_i, \nu_c$</td>
<td>Poisson’s ratio of the substrate, inclusion or coating</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Shear modulus</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>Kolosov constant</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Plastic zone size</td>
</tr>
<tr>
<td>$\rho^\perp, \rho^\parallel$</td>
<td>Density of climb or glide dislocations</td>
</tr>
<tr>
<td>$\Omega_\phi, \Gamma_\phi$</td>
<td>Subdomain of the inclusion or crack</td>
</tr>
<tr>
<td>$\xi, \zeta, \phi$</td>
<td>Element index in $x$-, $y$- or $z$-axis</td>
</tr>
<tr>
<td>$\Delta_x, \Delta_y, \Delta_z$</td>
<td>Half width of element</td>
</tr>
</tbody>
</table>
Chapter 1 Introduction

With the rapid development of complex manufacturing or utilization processes, microdefects are often formed and have important influences on the mechanical properties of materials, and may eventually result in material damages and structural failures. Therefore, it is of significance to understand the mechanisms of engineering components containing microdefects in order to improve their reliability and functionality for aerospace, automotive and medical applications. In this chapter, a brief introduction is firstly conducted on the mechanical properties of materials. Afterwards, the motivations and objectives for the study of the micromechanics of materials with defects are illustrated. Finally, the organization of the whole dissertation is presented.

1.1. Background

Mechanics of materials is a very fundamental subject for engineers. This subject is beneficial to the material design and can provide the safety analysis for different kinds of the mechanical and structural systems, such as airplanes, ships, buildings, bridges, machines, and spacecraft. An excellent understanding of the mechanical behaviors of materials is extremely important for their safe design. The fundamental concepts of mechanics mainly contain: the relationship between stresses and strains, deformation processes, displacements caused by the deformation, elasticity and inelasticity, strain energy, and loading/unloading paths. The main purpose of the mechanics is to determine the relationships among stresses, strains, and displacements in the materials due to the external loading subjected to them. These relationships can be affected by many factors, such as loading
conditions, defects, coating materials, temperatures, and lubrications. If these relationships can be expressed or predicted, we can obtain a clear picture of the mechanical behaviors of materials and effectively avoid their failure.

Commonly, materials experience a complex deformation process when they are subjected to the external forces. As one of the most widely used metals, the structural steel can be found in buildings, cranes, ships and many other fields. Its typical strain-stress diagram is considerable complex as shown in Fig. 1.1. It can be found that the steel begins with a linear proportional process (OA). This region is called elastic deformation and it will vanish instantaneously as soon as the external forces are removed. Brittle materials such as glass, ceramic, concrete or rocks only have elastic deformation before failure. With the increment of stress beyond point A, the strain begins to increase more rapidly for each increment in stress until point B. After this point, materials undergo a yield process (BC), which is known as perfectly plastic region and means the stress keeps unchanging with the increment of strain in the applied load. Then, a strain-hardened region (CD) appears and subsequently materials will fracture (DE and DE’). The region between points B and D is called plastic deformation and this process is irreversible or permanent.

Due to the complexity of the deformation process in the materials, many previous studies have mainly investigated their mechanical behaviors by analyzing the elastic properties [1-3]. However, the obtained results might not be very accurate since there are many metals that can undergo the substantially plastic deformation before they fail under a high pressure. As a result, many works have been conducted to study the elastic-plastic behaviors of the homogeneous materials in the past years [4-6].
However, microdefects such as cracks, voids and inclusions are often formed in materials during their manufacturing or utilization processes. They have significant influences on the material properties, including the mechanical properties, thermal properties, physical properties, etc. For example, inclusions often cause the stress concentrations, which might act as the sources of crack initiation and lead to the crack propagation. The presence of these microdefects may eventually result in material damages and structural failures. On the other hand, inclusions as the reinforcements can be added into composite materials to have excellent properties, which cannot be achieved by individual constituent materials [8]. Therefore, it is obviously that the effect of the same microdefect can be different and it depends on the detailed stress distribution of materials.

In order to further improve the investigations of materials with microdefects, the micromechanics is proposed to relate the mechanics and microstructures of materials [9]. This concept is widely used in the subsequent mechanics.

Fig. 1.1. The stress-strain diagram for a typical steel under the tensile loading [7].
investigations of inhomogeneous materials. A powerful and unified approach is proposed to solve these investigations, called the eigenstrain method. In term of the eigenstrain, it is a generic name and denotes nonelastic strains, including the thermal expansion, phase transformation, misfit strains, etc. This method has been used in the pioneer work about the inhomogeneity by Eshelby [10]. Then, he proposed the Equivalent Inclusion Method (EIM) to solve the elastic field of an infinite matrix with an ellipsoidal inhomogeneity. Afterwards, a larger number of works have been conducted to solve the inhomogeneous problems based on this method [11-15]. Recently, a detailed summary of the inhomogeneous problems has been done by Zhou et al. [16]. Moreover, cracks can be considered as a special case of voids. Different types of cracks, such as Zener-Stroh crack, Griffith crack and arc-shaped crack, have been investigated by many researchers. Bilby [17] firstly proposed to use the continuous distribution of dislocations to model and analyze various crack problems. This simulation method to model the crack is called the Distributed Dislocation Technique (DDT). A large number of numerical solutions to solve the crack problems based on this technique were summarized in [18].

The investigations of the elastic-plastic fracture behaviors of materials with cracks could date back to 1960s. For example, Arthur and Blackbur [19] studied the distribution of stresses and displacements for an elastic-perfectly plastic material with a single crack under the antiplane strain. Generally, the stresses at crack tips are predicted as infinite according to the linear elastic analysis. However, this prediction might not be accurate since the crack tips cannot be perfectly sharp. Therefore, Irwin model [20] and Dugdale model [21] were proposed to modify the crack tip stresses and they were the earliest two theoretical models focused on the plastic zone of crack tips. Irwin model was usually used to estimate the extent ahead
of a crack tip. This extent denoted the boundary between elastic and plastic regions and its size was determined by assuming the crack tip stress to the yield stress of the matrix material. Dugdale model assumed the plastic zone of crack tips was a thin strip and its size could be determined by canceling the stress intensity factor (SIF) due to the applied load and that due to the closure stress. Afterwards, these two models were fully developed and extended to solve the crack problems under different conditions [22-24]. For example, Hon et al. [25-28] used the modified Irwin or Dugdale models to investigate the plastic zone sizes and crack tip opening displacements (CTODs) for a crack interacting with different types of inclusions in an infinite space.

Though many previous studies have investigated the elastic behaviors or plastic behaviors of an infinite space with one crack and one inclusion, it should be noted that the interaction among different kinds of defects can significantly influence the mechanical properties of materials. This interaction should be taken into consideration in the mechanics investigation. Moreover, the complex external loading forces are usually applied to the engineering components, which would make the mechanics analysis more complicated.

Therefore, investigations of the micromechanics of solid materials with defects under various loading conditions are very important, and can improve the comprehensive understanding of the mechanical properties and promote the wide applications of materials.

1.2. Motivations

The deformation without considering the time effect could be mainly classified into two stages: elastic and plastic deformation stages. So far, a growing number of
studies have been conducted to investigate the elastic property of materials based on the Hooke’s law. However, few investigations have been done on the plastic behaviors of materials, which commonly exist in most of materials and can be influenced by many factors, such as the microdefects, types of idealized models, temperature and loading conditions. The accurate modelling of these factors plays a significant role in determining the mechanical properties of materials. For example, the stress ahead of crack tips changes dramatically when the materials are subjected to external forces. While this stress value is infinity in theory, it is difficult to be modeled in the numerical simulations and has significant influences on the mechanics analysis. Therefore, much attention should be paid to the investigations of the elastic-plastic behaviors of materials with defects.

Moreover, due to the complexity of experimental approaches, the plastic deformation problems are studied by using numerical modelling methods, such as the finite element method (FEM) and the discrete element method. These two methods are widely used to investigate the mechanical properties of materials. However, when considering the existence of microdefects in materials, numerous computational steps and a finer discretization are needed, which makes the computational process time-consuming. The high simulation time is a serious waste for the mechanics investigations of materials. Recently, a newly developed semi-analytic solution that combines the EIM and the DDT is proposed to simulate the elastic properties of materials with cracks and inhomogeneous inclusions [29]. In this solution, a modified conjugate gradient method (CGM) is proposed to solve the governing equations and a fast Fourier transform (FFT) algorithm is utilized to enhance the efficiency of the computational process. This solution can deal with the inhomogeneous problem quickly compared with other simulation methods.
1.3. Objectives

The present research works are focused on the micromechanics of defects in solid materials by using the semi-analytic solution. The effects of plastic zones of cracks and plastic increments of materials on the stress distribution are considered. The main objectives of the present research works are set as follows:

- To develop a semi-analytic solution to investigate the elastic-plastic fracture behaviors of an infinite space with cracks interacting with inhomogeneous inclusions, according to the modified Dugdale model;
- To study the elastic-plastic fracture behaviors of a half-space with cracks subjected to the prescribed pressure and contact loading;
- To investigate the elastic-plastic behaviors of a film-substrate with inhomogeneous inclusions subjected to contact loading;
- To study the elastic-plastic behaviors of a half-space with inhomogeneous inclusions and cracks subjected to contact loading;
- To provide guidance for the applications of materials with microdefects under the external loading.

1.4. Layout of the thesis

This PhD dissertation contains seven chapters. Following this introduction chapter, a literature review about the mechanics of materials, defects, modelling methods, crack-tip plasticity models, and contact problems is conducted. Chapter 3 illustrates the investigation of fracture behaviors of an infinite space with cracks and inhomogeneous inclusions under the remote stress. In Chapter 4, the study focuses on the fracture behaviors of a half-space with cracks subjected to the prescribed pressure or contact loading. Chapter 5 presents the influences of coating materials
and inhomogeneous inclusions on the elastic-plastic deformation of a film-substrate material subjected to contact loading. Chapter 6 deals with the influences of different cracks in a half-space material subjected to contact loading on the elastic-plastic behavior of materials. Chapter 7 concludes the main achievements of this dissertation and provides recommendations for future works.
Chapter 2 Literature Review

Mechanical properties are important to predict the material damages and structure failures. However, investigations of these properties are a very complex and difficult process. Due to the effect of manufacturing and utilization processes, most components are heterogeneous materials, such as composites, solid foams and polycrystals, which contain several kinds of microdefects. In order to have a better understanding of the mechanical properties of heterogeneous materials, the subject of micromechanics is proposed to relate the mechanics to microstructures of materials. This subject is based on the continuum theory of solid materials that contain microdefects. Therefore, it is of significance to understand the effects and micromechanics of defects in solid materials in order to improve the reliability and functionality of engineering components. In this chapter, the basic concepts of solid mechanics are firstly introduced. Then a review is conducted on the defects and their modeling methods. Afterwards, the investigation methods for the crack-tip plasticity and contact problems are reviewed. Finally, this chapter is summarized.

2.1. Fundamentals of solid mechanics

The solid mechanics of materials is usually complex in practical problems. Generally, it could be mainly classified into three stages. The first one, which is called elastic stage, is reversible and time-independent. In other words, the elastic deformation will vanish instantaneously as soon as the external forces are removed. A brittle material such as glass, ceramic, concrete or rocks can only have elastic deformation before failure. The deformation beyond the point of yielding, which is not strongly time dependent and irreversible/permanent, is called plastic.
deformation. After this stage, materials will fracture or damage and these results commonly occur induced by a large deformation or crack propagation. The detailed introduction of the basic concepts of solid mechanics will be reviewed following these three stages.

2.1.1. Elastic mechanics

Elastic property can be commonly found in many structural materials, including most metals, wood, plastics and ceramics. When they exhibit the linear elastic behavior under the tension or compression loading, the relationship between the stress $\sigma$ and the strain $\varepsilon$ can be expressed according to the Hooke’s Law:

$$\sigma = E\varepsilon,$$

(2.1)

where $E$ is a constant of proportionality. It indicates the modulus of elasticity for the materials. This modulus is also called Young’s modulus according to the scientist Thomas Young.

Hooke’s law can be extended to the three-dimensional case for isotropic materials. The detailed expressions are written as

$$\varepsilon_{xx} = \frac{1}{E} \left[ \sigma_{xx} - \nu (\sigma_{yy} + \sigma_{zz}) \right], \quad \gamma_{xy} = \frac{1}{G} \tau_{xy},$$

$$\varepsilon_{yy} = \frac{1}{E} \left[ \sigma_{yy} - \nu (\sigma_{xx} + \sigma_{zz}) \right], \quad \gamma_{yz} = \frac{1}{G} \tau_{yz},$$

(2.2)

$$\varepsilon_{zz} = \frac{1}{E} \left[ \sigma_{zz} - \nu (\sigma_{yy} + \sigma_{xx}) \right], \quad \gamma_{xz} = \frac{1}{G} \tau_{xz},$$

where $\nu$ is the Poisson’s ratio, $G$ is shear modulus; $\tau$ is the shear stress; and $\gamma$ is the shear strain.

In the real cases, most materials are heterogeneous due to the presence of inclusions, dislocations, disclinations and so on. These material discontinuities have significant influence on the elastic fields. In order to solve the heterogeneous
problems, the concept of eigenstrains was introduced by Mura [9]. Eigenstrain is a
generic name to denote the nonelastic strains, such as thermal expansion, phase
transformation, initial strains, plastic deformation, and misfit strains. Eigenstress is
caused by one or several of these eigenstrains. For the heterogeneous problems,
Hooke’s Law can be expressed as the following form:

\[ \sigma_{ij} = C_{ijkl}(\varepsilon_{kl} - \varepsilon^*_kl) \quad (i, j, k, l = 1, 2, 3), \] (2.3)

where \( C_{ijkl} \) are the elastic moduli and are constants; \( \varepsilon_{kl} \) is the elastic strain; and
\( \varepsilon^*_kl \) is the eigenstrain. In the tensor form, it should be noted that this Eq. (2.3)
contains six equations due to the shear stress \( \sigma_{ij} = \sigma_{ji} \) (\( i, j = 1, 2, 3 \)).

2.1.2. Plastic mechanics

Plastic deformation of materials is a very complex process in the real cases.
This process can be influenced easily by many factors, such as the loading history,
yield condition, working-hardening, microstructure, and so on. The original works
of plasticity date back to a series of papers by Tresca on the extrusion of metals in
1864 and von Mises on the general plastic equations in 1913. Afterwards, many
mathematical and numerical methods based on their works were proposed to
investigate the plastic behaviors of materials.

In order to simplify the plastic behaviors of the real materials, one can idealize
the plastic models of materials [30-32]. The most commonly used models are shown
in Fig. 2.1. The choice of different models depends on the actual applications. For
example, if the deformation body is the mild steel, the working-hardening effect
could be neglected according to the experimental results. In this case, the perfectly
plastic model is more accurate (Fig. 2.1 (c)).
Fig. 2.1. The stress-strain curves of the commonly used elastic-plastic models: (a) rigid-perfectly plastic material, (b) rigid-perfectly linear hardening material, (c) elastic-perfectly plastic material, (d) elastic-linearly hardening material, and (e) elastic nonlinear plastic material.

For the numerical simulation methods, the yield criterions, flow rules, strain hardening rules and the loading-unloading conditions are of significance for the plastic mechanism of materials [33]. Generally, when the material yields, the stress state can be determined according to different yield criterions. After the yield occurs, the increment of the plastic strain need to be calculated according to the flow rules and strain hardening laws. The loading-unloading conditions are commonly used to determine the subsequence yield situations in the loading process. The detailed information of the yield criterions, flow rules, strain hardening rules and loading paths will be summarized as follows.

Generally, for the materials without the critical yield point, it is difficult to find a threshold below which there is only pure elastic deformation. However, for the materials that have critical yield points, it is normal to define the yield stress that
Chapter 2 Literature Review

separates the elastic and plastic regions. There are two widely used yield criteria: the von Mises yield criterion and the Tresca yield criterion.

The first criterion uses the elastic shear energy density to determine the threshold of elastic behaviors. In other words, when the second invariant of the deviatoric stress tensor approaches a critical value, the yield of material will occur. It is represented by principle stresses as follow:

\[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_1 - \sigma_3)^2 = 2\sigma_Y^2, \quad (2.4)\]

where \(\sigma_1, \sigma_2\) and \(\sigma_3\) are the principle stresses; and \(\sigma_Y\) is the yield strength.

The second criterion is based on another assumption. It denotes that when the maximum shear stress exceeds a critical value, the elastic threshold is reached. According to the principal stresses, it can be written as

\[
\max [|\sigma_1 - \sigma_2|, |\sigma_2 - \sigma_3|, |\sigma_1 - \sigma_3|] = \sigma_Y. \quad (2.5)
\]

The yield surfaces of these two criteria for the plane stress condition and the three-dimensional principle stress space are shown in Figs. 2.2 and 2.3, respectively. It is obvious that the ellipse curve represents the Mises yield surface and the hexagon one represents the Tresca yield surface.

![Diagram](image)

**Fig. 2.2.** The yield surfaces of von Mises and Tresca yield criterions for plain strain condition.
For the plastic deformation, a very important feature, compared with elastic deformation, is the history-dependent or path-dependent nature, which requires that the constitutive equations for the plastic deformation could be in differential equations or incremental forms. Commonly, two kinds of flow rules can be used to describe the increment of plastic strain: Levy-Mises equations and Prandtl-Reuss equations. The first rule assumes that the elastic strain is so small as to be negligible and the increment of strain is coaxial with the deviatoric stress. It can be written as

\[ d\varepsilon_{ij} = d\lambda\sigma'_{ij}, \]  

(2.6)

where \( \lambda \) is a scalar factor of proportionality.

The second rule states that the total strain increment can be obtained by summing the elastic strain and plastic strain increments. The detailed equation could be written as
\[
\delta \varepsilon_{ij} = \delta \varepsilon_{ij}^e + \delta \varepsilon_{ij}^p \quad \text{with} \quad \delta \varepsilon_{ij}^p = d \lambda \sigma_{ij},
\]  
(2.7)

where \( d \lambda \) is the effective plastic incremental strain. In order to calculate the result of \( d \lambda \), a universal integration algorithm is developed for the elastoplastic materials with hardening effects by Fotiu et al. [34]. However, this method seems not very stable and accurate. Then, Nelias and NematNasser [35] proposed an algorithm to improve the convergence of plasticity loop. Based on their idea, Chen et al. [6] combined it with the Newton-Raphson iteration scheme to develop a solution for calculating the plastic strain increment. This solution was used in this study to investigate the elastic-plastic behaviors of materials with defects.

Furthermore, the plastic deformation can also be influenced by the strain hardening rules, which could be mainly classified into three types: no strain hardening, linear strain hardening and nonlinear strain hardening. For the linear model, the formula is simple and only an appropriate value needs to be chosen to represent the slope of hardening effect. However, for the nonlinear model, it is difficult to determine a unique expression to describe the model. Therefore, many equations for the nonlinear working-hardening effect have been proposed in the last century, which are summarized in Table. 2.1.

Currently, many methods are used to investigate the plastic behaviors of homogeneous materials [36-40]. A elastic-plastic contact code was proposed by Jacq et al. [4] to solve the three-dimensional problem. When considering the plastic strain, they obtained a closed form expression for the residual stresses and surface displacements. These obtained results had been validated by comparing them with the nano-indentation results. Wang and Keer [41] used a CGM and a fast convergence to improve the computational efficiency for the above mentioned code. Afterwards, this contact code was extended to analyze the plastic effect under the
repeated loading according to different hardening laws [42] and then investigate the elastic-plastic behaviors of a layered materials in indentation [43]. This code also provides a fundamental reference to the subsequence works focused on the elastic-plastic investigation of materials with microdefects.

**Table 2.1 Equations of materials with nonlinear working-hardening.**

<table>
<thead>
<tr>
<th>Equations for nonlinear working-hardening</th>
<th>Researchers</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma = \sigma_y + H \varepsilon^n$</td>
<td>Ludwick</td>
<td>1909</td>
</tr>
<tr>
<td>$\sigma = H \varepsilon^n$</td>
<td>Holloman</td>
<td>1944</td>
</tr>
<tr>
<td>$\sigma = \sigma_y + (\sigma_y - \varepsilon){1 - \exp(-n\varepsilon)}$</td>
<td>Voce</td>
<td>1948</td>
</tr>
<tr>
<td>$\sigma = H(\varepsilon_y + \varepsilon)^n$</td>
<td>Swift</td>
<td>1947</td>
</tr>
<tr>
<td>$\sigma = \sigma_y \tanh\left(\frac{E}{E_y}\right)$</td>
<td>Prager</td>
<td>1938</td>
</tr>
<tr>
<td>$\sigma = \frac{\sigma}{E} + H\left(\frac{\sigma}{E}\right)^n$</td>
<td>Ramberg and Osgood</td>
<td>1943</td>
</tr>
</tbody>
</table>

**2.1.3. Fracture mechanics**

Engineering components are commonly subjected to different loading conditions, such as tension, compression, bending, torsion, or combinations of them. These complex loading conditions may easily cause the material to fracture, especially for the materials with defects [44]. For example, due to the presence of cracks in a component material, it might fail when the stresses are below the yield strength. Since the cracks are difficult to avoid in materials, the linear elastic fracture mechanics is proposed and widely used to investigate and predict the crack problems by considering the stress, geometry and crack size.

The original fracture mechanics was used to analyze a continuum material with
an a-priori defect with the length $a$. It indicates that this material will fracture when their stress approaches a critical value $\sigma_C$, which can be expressed by

$$\sigma_C = \frac{K_C}{Y(\pi a)^{1/2}},$$

where $K_C$ is the intensity factor of critical stress and $Y$ is a geometric factor.

The early work related the fracture stress and flaw size was conducted by Griffith, who also introduced the concepts of the stress intensity parameters and energy release rate [45]. Then, he predicted the crack growth based on the energy balance and concluded that the crack would grow when the induced energy was enough to create the new crack surface. In 1956, Irwin proposed an energy approach for fracture based on the energy rate $G$. It can be expressed as the negative of the derivative of potential energy corresponding to the crack area:

$$G = -\frac{d\Pi}{dA},$$

where $A$ is the crack area and $\Pi$ is the potential energy. This energy should be changed with the energy required to generate the new crack surface.

In the early 1960s, Paris et al. [46, 47] presented that the fracture mechanics was a useful tool to investigate the crack growth by fatigue. Since that time, the fracture mechanics has been widely used to solve the propagation problems of fatigue cracks. Generally, researchers use the ratio between the crack growth per cycle of loading $da/dN$ against the range of stress intensity factor $\Delta K = K_{\text{max}} - K_{\text{min}}$ to describe the propagation of fatigue crack. The typical fatigue crack growth behaviors are mainly classified into three regions. In the region I, the value of $\Delta K$ is smaller than the threshold $\Delta K_{\text{th}}$, which means that it is difficult for the crack to propagate. In the region II, the ratio between $da/dN$ and $\Delta K$ is almost linear. In the region III, the crack growth rate can accelerate as $K_{\text{max}}$ reaches $K_C$, the
fracture toughness of the specific material. This linear relationship in the region II can be described firstly by a power law proposed by Paris and Erdogan [47] as follow:

\[ \frac{da}{dN} = C\Delta K^m, \]  

(2.10)

where \( C \) and \( m \) are material constants. They are usually determined by the experimental method.

Afterwards, this equation was modified by Klesnil and Lukas to study the fatigue crack propagation problems considering the threshold \( \Delta K_{th} \) [48, 49]. It should be noted that the crack growth and propagation can highly influence the fracture properties of materials.

### 2.2. Defects in solid materials

Defects are easily formed during the manufacturing or utilization processes in the engineering components. Commonly, they have different types in the real materials. Due to the existence of defects, the properties and deformation mechanics of materials can be changed significantly. In this part, we just focus on the dislocations, cracks and inclusions. A brief review of these defects and the research situations will be conducted. These defects can interact with each other and the works about the interaction are also reviewed.

#### 2.2.1. Dislocations

The dislocation is a kind of crystallographic defects or irregularities on the atomic scale and can be classified by the edge, screw and mixed dislocations (or classified by perfect and partial dislocations). As shown in Fig. 2.4(a), the edge dislocation is imagined as the border of an extra plane of atoms. For the screw
dislocation, it can be regarded by cutting a perfect crystal along a plane and slipping one half across the other as shown in Fig. 2.4(b). Generally, dislocations in solids have a combined form with the edge and screw types simultaneous. In most situations, the Burgers vector \( b \) can describe the magnitude and direction of the lattice distortion resulting from a dislocation in a crystal lattice. When it is parallel or perpendicular to the dislocation line, the corresponding dislocation is edge or screw type.

![Fig. 2.4](image)

**Fig. 2.4.** The two basic types of dislocations in the crystal structure: (a) edge dislocation, and (b) screw dislocation.

For the edge dislocations, there are two ways to produce them with a Burgers \( b_x \). As shown in Fig. 2.5(a), it can be considered that a cut is made along the positive \( y \)-axis and then pull the material separated. Then a thin trip of thickness \( b_x \) is inserted before re-joining. The climb edge dislocation is formed using this method. For the creation of the glide edge dislocation, it can be imaged that a cut along the positive \( x \)-axis is made firstly and then slip the material below the cut in the \( x \)-direction by an amount \( b_x \) before re-joining, as shown in Fig. 2.5(b). When the relative displacement between the materials on both sides of the cut is a constant in the \( x \)-direction, the induced stress fields and displacements in the \( y \)-direction are the
Chapter 2 Literature Review

same for both dislocated bodies. Moreover, the dislocation can be defined as climb dislocation when its $b_x$ is perpendicular to the path cut, just like in Fig. 2.5(a). If the $b_x$ is parallel to the path cut, it can be regarded as glide dislocation and this will induce shear displacements.

![Diagram of dislocations](image)

(a) The climb edge dislocation  (b) The glide edge dislocation

**Fig. 2.5.** The creation of an edge dislocation.

The slip of dislocations can significantly influence the plastic behaviors of materials, especially when the metals undergo the work hardening and annealing processes. In 1934, Taylor and other two researchers found that the plastic deformation could be explained using the theory of dislocations at the same time [50]. Afterwards, Stngni and Lizzio [51] and Tsuchida et al. [52] developed a solution to investigate the elastic interaction between an elliptical inhomogeneity and an edge dislocation. Due to the manufacturing processes, the dislocations can interact with the inhomogeneities and then affect the hardening, strengthening, and toughening effects of materials. Therefore, much attention has been focused on this interaction. Shodja et al. [53] focused on the elastic behaviors and size effects of an edge dislocation, which was outside an elliptical inhomogeneity. It was found that the normalized image force was highly depending on the size of the inhomogeneity. Fang et al. [54, 55] investigated the interaction between the dislocations and circular inhomogeneity and considered the interface effect. Luo and Xiao [56] investigated
the image force between an elliptical inhomogeneity and a screw dislocation in an infinite space material. Fan et al. [57] investigated the fracture behaviors for edge dislocations interacting with a inhomogeneity. This interaction between dislocations and inhomogeneity was also studied in many other works [58-63].

2.2.2. Cracks

As can be seen in Fig. 2.6, an edge crack can experience three types of loadings: Mode I (opening mode), Mode II (in-plane shear mode), and Mode III (out-of-plane shear, or tearing mode). Commonly, cracks may be subjected to any one of these modes, or a combination of two or three modes. When a crack experiences a combined loading mode, it means to be under mixed mode loading. In fact, most engineering components are subjected to the mixed mode loading. In addition, the resistance of a material subjected to different cracking modes is diverse. This resistance can be represented by the value of the fracture toughness. Generally, the value for Mode I crack is higher than that for Modes II and III. However, this might be changed especially for the composite materials since they have internal structures with anisotropic mechanical properties.

![Mode I, Mode II, Mode III](image)

**Fig. 2.6.** The three modes of the loading condition that can be applied to a crack.
Considering the plane state problems, the fields of the stress and displacement due to the crack with a length of 2a will be calculated by defining the origin at one of the crack tip in the polar coordinate axis. The detailed expressions for these two fields according to Modes I and II are expressed in Tables 2.2 and 2.3, respectively.

**Table 2.2 Stress fields ahead of a crack tip for Modes I and II [30].**

<table>
<thead>
<tr>
<th>Mode I</th>
<th>Mode II</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sigma_{xx} = \frac{K}{\sqrt{2\pi r}} \cos \left( \frac{\theta}{2} \right) \left[ 1 - \sin \left( \frac{\theta}{2} \right) \sin \left( \frac{3\theta}{2} \right) \right] )</td>
<td>( \sigma_{xx} = -\frac{K}{\sqrt{2\pi r}} \sin \left( \frac{\theta}{2} \right) \left[ 2 + \cos \left( \frac{\theta}{2} \right) \cos \left( \frac{3\theta}{2} \right) \right] )</td>
</tr>
<tr>
<td>( \sigma_{yy} = \frac{K}{\sqrt{2\pi r}} \cos \left( \frac{\theta}{2} \right) \left[ 1 + \sin \left( \frac{\theta}{2} \right) \sin \left( \frac{3\theta}{2} \right) \right] )</td>
<td>( \sigma_{yy} = -\frac{K}{\sqrt{2\pi r}} \cos \left( \frac{\theta}{2} \right) \sin \left( \frac{\theta}{2} \right) \cos \left( \frac{3\theta}{2} \right) )</td>
</tr>
<tr>
<td>( \tau_{xy} = \frac{K}{\sqrt{2\pi r}} \cos \left( \frac{\theta}{2} \right) \sin \left( \frac{\theta}{2} \right) \cos \left( \frac{3\theta}{2} \right) )</td>
<td>( \tau_{xy} = \frac{K}{\sqrt{2\pi r}} \cos \left( \frac{\theta}{2} \right) \left[ 1 - \sin \left( \frac{\theta}{2} \right) \sin \left( \frac{3\theta}{2} \right) \right] )</td>
</tr>
<tr>
<td>( \sigma_{zz} = \begin{cases} 0 &amp; \text{(plane stress)} \ \nu(\sigma_{xx} + \sigma_{yy}) &amp; \text{(plane strain)} \end{cases} )</td>
<td>( \sigma_{zz} = \begin{cases} 0 &amp; \text{(plane stress)} \ \nu(\sigma_{xx} + \sigma_{yy}) &amp; \text{(plane strain)} \end{cases} )</td>
</tr>
<tr>
<td>( \tau_{xz} = \tau_{yz} = 0 )</td>
<td>( \tau_{xz} = \tau_{yz} = 0 )</td>
</tr>
</tbody>
</table>

**Note:** \( K \) is a characterization constant which depends on crack geometry and loading and boundary condition; and the Poisson’s ratio is denoted by \( \nu \).

**Table 2.3 Crack-tip displacement fields for Modes I and II [30].**

<table>
<thead>
<tr>
<th>Mode I</th>
<th>Mode II</th>
</tr>
</thead>
<tbody>
<tr>
<td>( u_x = \frac{K}{2G} \sqrt{\frac{r}{2\pi}} \cos \left( \frac{\theta}{2} \right) \left[ \kappa - 1 + 2\sin^2 \left( \frac{\theta}{2} \right) \right] )</td>
<td>( u_x = \frac{K}{2G} \sqrt{\frac{r}{2\pi}} \sin \left( \frac{\theta}{2} \right) \left[ \kappa + 1 + 2\cos^2 \left( \frac{\theta}{2} \right) \right] )</td>
</tr>
<tr>
<td>( u_y = \frac{K}{2G} \sqrt{\frac{r}{2\pi}} \sin \left( \frac{\theta}{2} \right) \left[ \kappa + 1 - 2\cos^2 \left( \frac{\theta}{2} \right) \right] )</td>
<td>( u_y = -\frac{K}{2G} \sqrt{\frac{r}{2\pi}} \cos \left( \frac{\theta}{2} \right) \left[ \kappa - 1 - 2\sin^2 \left( \frac{\theta}{2} \right) \right] )</td>
</tr>
<tr>
<td>( u_z = \frac{K}{2G} \sqrt{\frac{r}{2\pi}} \cos \left( \frac{\theta}{2} \right) \left[ \kappa + 1 - 2\sin^2 \left( \frac{\theta}{2} \right) \right] )</td>
<td>( u_z = -\frac{K}{2G} \sqrt{\frac{r}{2\pi}} \sin \left( \frac{\theta}{2} \right) \left[ \kappa - 1 + 2\cos^2 \left( \frac{\theta}{2} \right) \right] )</td>
</tr>
</tbody>
</table>

**Note:** \( \kappa \) is a Kolosov constant and \( G \) is the shear modulus.
The stress intensity factor is a very important parameter of cracks. Similar to the loading modes, the SIFs also have three forms $K_I$, $K_{II}$ and $K_{III}$, representing the Modes I, II and III, respectively. When the stress components of materials with cracks are obtained, the expressions for the three types of SIFs crack can be written as follows:

\[
K_I = \lim_{r \to 0} \left( \sqrt{2 \pi r} \sigma_{yy} \right), \tag{2.11a}
\]

\[
K_{II} = \lim_{r \to 0} \left( \sqrt{2 \pi r} \tau_{xy} \right), \tag{2.11b}
\]

\[
K_{III} = \lim_{r \to 0} \left( \sqrt{2 \pi r} \tau_{yz} \right), \tag{2.11c}
\]

where the factor of $\sqrt{2 \pi}$ is included according to convention.

Moreover, the SIFs can be influenced by many factors, such as crack types, crack numbers and positions, loading conditions and finite sizes of the materials. Several books explained and summarized the solutions to obtain the SIFs for different configurations [64-66].

Generally, cracks are initiated at the positions of high stress concentrations. The formation and growth of cracks have been widely investigated in many works by the molecular statics or molecular dynamics simulations [67-70]. For example, the Zener-Stroh crack is induced through the dislocations stopped by an inclusion, which was firstly proposed by Zener. This kind of crack has a finite opening displacement at one end and a zero displacement at the other end. Afterwards, Stroh [71] studied the stress concentration round the plied-up of dislocations at the end of a slip line and judged whether it was sufficient to initiate a crack. Moreover, disclinations may be unstable and act as the sources of crack nucleation. The first model used to investigate this crack formation was proposed by Rybin and Zhukovskii [72]. In fact, many ways may induce or initiate the crack and cause
propagation. This also indicates that the interaction between different defects is complicated and needs further investigations.

2.2.3. Inclusions

Inclusions commonly exist in engineering components, which can significantly influence the stress distribution around them and affect the mechanical properties of materials. For example, inclusions can be added into the composite materials as reinforcements to obtain the excellent properties, compared with the corresponding constituent material. Moreover, the presence of inclusions is inevitable in the material manufacturing processes. This might cause the stress concentrations easily and acts as the sources of crack initiation.

Based on the definition of Mura [9], there are three types of inclusions: the inhomogeneity, inhomogeneous inclusions, and homogeneous inclusions. Generally, the inhomogeneity has different elastic modulus than its surrounding material, which can be found in many engineering materials. Compared with the inhomogeneity, the inhomogeneous inclusion not only has the different elastic modulus from the matrix material but also contains eigenstrains. For the homogeneous inclusion, it has the same elastic modulus as the matrix material but contains eigenstrains.

Recently, many investigations have been conducted on mechanical properties of materials with different shapes of inhomogeneous inclusions, such as a circular rigid disc [73], an embedded ellipsoidal inhomogeneity [74], a hemispheroidal inhomogeneity [75], a prolate spheroidal inhomogeneous inclusion [76] and two concentric spherical inhomogeneities [77].

The problem of inclusions in an infinite space has also been investigated in
many works [15, 78] based on different methods. For example, Wang and Zhou [79] proposed a method based on the analytical continuation and conformal mapping to investigate an infinite or semi-infinite two-dimensional problem with arbitrarily shaped inclusion. However, unlike the inclusions in an infinite space material, the problems of them in a half-space are of significance since the high pressure at the free surface might cause the seriously stress concentrations especially when the inclusions are near this free surface. Therefore, many approaches were applied to solve the half-space problem with inhomogeneous inclusions, including an ellipsoidal inclusion [80], a spheroidal inclusion [81], a hollow cylindrical inclusion [82], a cuboidal inclusion [83], a hemispherical inclusion [84], and a solid cylindrical inclusion [85]. Generally, the contact loading applied between two bodies might make the half-space problem more complicated since the unknown surface contact pressure and area need to be calculated firstly. Kuo [86, 87] used the boundary element method to study the stress disturbances caused by a single or multiple inhomogeneities in a half-space material under contact loading. It can be found that the inhomogeneities have significant influence on the contact pressure and shear stress distributions.

2.3. Modelling of defects

2.3.1. Distributed dislocation technique

According to the previous works done by Eshelby, Keer, Erdogan, Mura and many others, the DDT was proposed to solve the crack problems in many real cases. The basic idea of this technique is to use the unknown distribution of the dislocation densities to model cracks and then superpose the stress field in the homogeneous space. These unknown densities can be determined when the crack faces satisfy the
traction-free condition.

The detailed information of this technique will be introduced based on the plane problem. Fig. 2.7 (a) illustrates a plane crack with the length $2a$ embedded in an infinite space under the remote tensile stress. According to the Bueckner’s theory, this inhomogeneous plane problem could be transformed into two sub-problems. The first one is the stresses induced by the uncracked body as shown in Fig. 2.7 (b). The other one is the stresses caused by the unloaded body as shown in Fig. 2.7 (c). Based on the superposition, the total stresses can be obtained by

$$\sigma_{ij}(x, y) = \tilde{\sigma}_{ij}(x, y) + \hat{\sigma}_{ij}(x, y),$$

(2.12)

where $\tilde{\sigma}_{ij}(x, y)$ is the stress induced in the absence of the crack and $\hat{\sigma}_{ij}(x, y)$ is the stress caused by adding materials to fill the crack without any external loading. This expression can be obtained when the boundary conditions are satisfied at infinity and at the traction-free crack faces simultaneously.

![Fig. 2.7. Decomposition for a plane crack opened by tension stress based on the Bueckner’s principle.](image)

Chapter 2 Literature Review
Based on the DDT, the crack can be molded by a distribution of dislocations with unknown densities along the lines where the crack originally appeared. The Modes I and II cracks can be treated as the climb and glide edge dislocations, respectively. Then, the mixed dislocations (containing climb and glide) are used to simulate the mixed Mode crack. Therefore, the stress $\sigma_{ij}$ at point $(x, y)$ induced by an edge dislocation with the Burgers vector components $b^\perp$ and $b^\parallel$ located at $(x^d, y^d)$ is obtained by

$$\sigma_{ij}(x, y, x^d, y^d) = \sigma_{ij}^\perp(x, y, x^d, y^d) + \sigma_{ij}^\parallel(x, y, x^d, y^d), \quad (i, j = 1, 2). \quad (2.13)$$

For the Griffith crack, $\sigma_{ij}^\perp$ and $\sigma_{ij}^\parallel$ can be represented as

$$\sigma_{ij}^\perp(x, y, x^d, y^d) = \frac{2\mu}{\pi(k + 1)} b^\perp(x^d, y^d) G_{ij}^\perp(x, y, x^d, y^d), \quad (2.14a)$$

$$\sigma_{ij}^\parallel(x, y, x^d, y^d) = \frac{2\mu}{\pi(k + 1)} b^\parallel(x^d, y^d) G_{ij}^\parallel(x, y, x^d, y^d), \quad (2.14b)$$

where $\mu$ is the shear modulus; $k$ is the Kolosov constant, which equals $3 - 4\nu$ for the plane strain problem; and $G_{ij}^\perp$ and $G_{ij}^\parallel$ are the influence functions.

The stresses induced by a single dislocation can be calculated by Eq. (2.14). When considering the dislocations alone the original crack line (used to model the crack), the stress field $\hat{\sigma}_{ij}(x, y)$ can be obtained by the integration of the stress field components $\sigma_{ij}(x, y, x^d, y^d)$:

$$\hat{\sigma}_{ij}(x, y) = \frac{2\mu}{\pi(k + 1)} \left[ \int_{-a}^{+a} \rho^\perp(x') G_{ij}^\perp(x, y, x^d - x', y^d) dx' \right] + \int_{-a}^{+a} \rho^\parallel(x') G_{ij}^\parallel(x, y, x^d - x', y^d) dx', \quad (2.15)$$

where $\rho^\perp(x)$ and $\rho^\parallel(x)$ are the dislocation densities. They can be obtained by satisfying the free traction condition ($\hat{\sigma}_{ij}(x, y) + \hat{\sigma}_{ij}(x, y) = 0$ along crack). Once the dislocation densities $\rho^\perp(x)$ and $\rho^\parallel(x)$ are obtained, the displacement across
the crack can be obtained by integrating them: $D(x) = -\int_{-a}^{x} \rho(x) \, dx$. For a Griffith crack, the crack faces must be closed at both crack ends, which means that there is no net dislocation resulting in zero sum of the dislocation density. It can be expressed as: $\int_{-a}^{a} \rho(x) \, dx = 0$.

Recently, this technique has been extensively applied to investigate the crack problems [88-90]. For example, Blomerus et al. [91] applied this method to analyze the elastoplastic strain concentrations and consider the influence of the boundary conditions. Codringron et al. [92] investigated the cyclic crack tip plasticity effects by this technique. The growth of a short crack in a crystal under the fatigue loading was studied by Hansson et al. [93]. Philipps et al. [94] investigated the crack tip stress intensity factors for a crack initiating from a sharp notch. Xiao et al. [95] analyzed the stress field considering a Zener-Stroh crack and a coated inclusion. The influence of the material constants, the distance between the inclusion and the crack, and the coating layer on the stress intensity factors was analyzed. Zhou et al. [96]. They used a semi-analytic solution to study the elastic stress field of the half-space material with cracks under contact loading. They derived the formula to obtain the coefficients relating the stress to dislocations and that relating the displacement to the dislocations based on this technique.

### 2.3.2. Equivalent inclusion method

According to the EIM proposed by Eshelby [10], an inhomogeneity or inhomogeneous inclusion could be considered as a homogeneous inclusion with initially prescribed eigenstrains plus equivalent eigenstrains. Fig. 2.8 (a) shows an ellipsoidal inhomogeneous inclusion $\Omega$ with elastic moduli $C_{ijkl}^\Omega$ and initial eigenstrain $\epsilon_{ij}^p$ in an infinite material $D$ with elastic moduli $C_{ijkl}^D$. By using this
approach, this inhomogeneous inclusion can be modeled as a homogeneous inclusion of elastic moduli $C_{ijkl}^D$ with $\epsilon_{ij}^P$ plus equivalent eigenstrain $\epsilon_{ij}^*$ as shown in Fig. 2.8 (b). In this ellipsoid, the equivalent eigenstrains $\epsilon_{ij}^*$ and stresses were found to be uniform when the initial eigenstrains $\epsilon_{ij}^P$ are uniform.

Since then, the EIM has been extensively used and extended to investigate the complex inclusion problems, including the solitary inclusion and multiple inclusions problems in the two-dimensional or three-dimensional matrix materials. The interaction among all the inclusions can be considered due to the equivalent eigenstrains.

At the beginning, this method was just used to solve the infinite space problems with the cubical inclusion [97], cylindrical inclusion [98] and strip inclusion [99]. Afterwards, it was used to study the multiple arbitrary shape inclusions by Zhou et al. [100]. They proposed a general and robust solution for this problem since five aspects were considered: a multiple number of inhomogeneous inclusions can be studied; the interaction among all the inclusions are taken into consideration; each inclusion has an irregular shape; the material in one inclusion can be different from that of the other, and the initial eigenstrain and applied loading can be non-uniform.

However, the problems of inclusions in a half-space are of more practical interest since many sites of initial strains caused by high stresses occur at the free surface. Unlike the inclusion problem in an infinite space, the surface effects cannot be neglected when the inclusions is near a free surface, especially for the contact surface. Therefore, the EIM was extended to study the half-space problems [74, 80, 83, 84, 101-103]. Zhou et al. [14] developed a semi-analytic solution to investigate elastic properties of the three-dimensional half-space with multiple inhomogeneous
inclusions. Moreover, with this method, the coating layer can be treated as an inclusion when two conditions are satisfied. The first one is that the length and width of the inhomogeneity must be larger than its thickness. The second one is that the length and width must be larger than the sizes of the contact area. Then, Zhou et al. [103] investigated the effect of stiff inclusions in a film-substrate on the elastic field. It was found that the stiff inhomogeneities in the substrate would not worsen the cracking and deboding of a hard coating and still have detrimental effect on the yield behaviors of the film-substrate materials.

![Diagram of inhomogeneous and homogeneous inclusions](image)

**Fig. 2.8.** The schematics for the original inhomogeneous inclusion problem (a) and the homogeneous problem by means of the EIM (b).

### 2.4. Crack-tip plasticity

The stresses at the sharp crack tips are predicted to be infinite based on the linear elastic analysis. However, they are finite in real materials since the radius of crack tips must be finite. Therefore, the elastic stress analysis is not very accurate when considering the influence of the stresses at crack tips. This inaccuracy will be improved by considering the influences of plastic zones ahead of the crack tips. The
two earliest used models to analyze and estimate the plastic zones of crack tips are the Irwin model and Dugdale model. Moreover, the plastic zone shape is another important parameter of the crack-tip plasticity. It can be determined according to the stress field and the yield criterion, which can be influenced by the plane strain or plane stress conditions. As a result, this section focuses on the research of two crack models and the plastic zone shape.

2.4.1. Dugdale model

The Dugdale model is also called the strip-yield model, which was proposed by Dugdale [21] and Barenblatt [104]. In this model, a slender strip of non-hardening plastic strip exists at either end of a crack, as shown in Fig. 2.9. They investigated a through crack in an infinite space and assumed that the plastic zone at the crack tips is a long and slender region. Therefore, the effective crack length is assumed to be $2a + 2\rho$, where $a$ is the original half crack length and $\rho$ is the length of the plastic zone. The infinite space is assumed as the non-hardening material with the closure stress $\sigma_{YS}$ applied at the crack plastic zones.

![Fig. 2.9. The plastic zones and yield stress distribution ahead of crack tips according to the Dugdale crack model.](image-url)
Since the stresses are finite at the plastic zones, a stress singularity cannot be found at the crack tips. Therefore, the plastic zone size of crack tips must be chosen such that the SIFs due to the remote tension and the closure stresses cancel each other:

\[ K_\sigma + K_{\text{closure}} = 0, \]  

(2.16)

where \( K_{\text{closure}} \) is the SIF due to the closure stress of the infinite material and \( K_\sigma \) is the SIF due to the applied remote tension.

The crack tip opening displacement (CTOD) is defined as the displacement at the original crack tip. It is a key parameter in fracture mechanics to judge whether a fracture will occur in solid materials. Moreover, it can also be used to determine the imminent crack extension by comparing it with a critical value. When the plastic strips are taken into consideration, the CTOD might have already reached the critical value. For the Dugdale model, a crack of length \( 2(a + \rho) \) with the yield strips occupying \( -(a + \rho) \leq x \leq -a \) and \( a \leq x \leq (a + \rho) \), where \( x \) is measured from the crack center, is considered. When a far field loading \( \sigma \) perpendicular to the crack plane is applied, the CTOD at the original crack tip \( (x = a \) and \( x = -a) \) can be obtained:

\[ \delta = \frac{8\sigma_y a}{\pi E} \ln \sec \left( \frac{\pi \sigma}{2\sigma_y} \right). \]  

(2.17)

where \( \sigma_y \) and \( E \) are the yield stress and Young’s modulus of the matrix material.

Based on the Dugdale crack model, Howard and Otter [105] investigated the elastic-plastic deformation of a sheet with an crack under the tensile loading according to the small scale yielding as well as asymptotic large scale yielding assumptions. Afterwards, Singh et al. [106] proposed a method to study the plastic
zones of circular edge cracks, which were located in a stretched cylinder. Bostrom [107] focused on the stress analysis in an infinite sheet with the consideration of the short radial cracks induced by a circular hole.

The model can also be applied to study the mixed mode loaded Dugdale crack problem, which was firstly proposed by Becker and Gross [108]. They also proposed the yield criterion along strips, and the overlapping of crack and strip faces. This mixed model is of great importance to analyze the mechanical problem of materials with cracks. Recently, Hoh et al. [25] used an analytical solution to investigate an infinite space problem with a crack and a circular inclusion. Based on the Erdogan and Gupta’ method, they studied the effect of the load-to-yield-stress ratio, the material constants, and the crack-inclusion distance on the CTOD and plastic zone size. Afterwards, Yi et al. [109] used the modified Dugdale model to investigate the plastic behaviors of an infinite bi-material plate with a sub-interface penny-shaped crack. This model was employed to solve the similar behaviors of a sub-interface Zener-Stroh crack by Fan et al. [110]. The studies based on this model can also be found in many other works [26, 28, 111-113].

2.4.2. Irwin model

In 1968, the Irwin model was proposed to estimate the elastic-plastic boundary, which was illustrated in Fig. 2.10. Considering the crack plane ($\theta = 0$), the normal stress $\sigma_{yy}$ in a linear elastic material can be given as $K_I/\sqrt{2\pi r}$, where $K_I$ represents the SIF of Mode I. The boundary condition between the elastic and plastic behaviors can be determined by satisfying the yield criterion: $\sigma_{yy} = \sigma_{YS}$, where $\sigma_{YS}$ is the uniaxial yield strength. Therefore, the first-order estimate of the plastic zone size $r_y$ can be obtained:
\[ r_y = \frac{1}{2\pi} \left( \frac{K_1}{\sigma_{ys}} \right)^2. \] (2.18)

However, this estimate is not strictly correct since it is based on the elastic crack tip solution. When the material is elastic-perfectly plastic (the strain hardening effect can be neglected), the stress singularity is truncated by yielding at the crack tip. The stresses must be redistributed in order to satisfy the equilibrium condition when the material yields. The forces represented by the cross-hatched region need to be accommodated by increasing the plastic zone size, since they cannot exceed the yield strength when considering the elastic-perfectly plastic material. Therefore, the second-order estimate of the plastic zone size \( r_p \) needs to satisfy the following force balance equation:

\[ \sigma_{ys} r_p = \int_0^{r_y} \sigma_{yy} dr = \int_0^{r_y} \frac{K_1}{\sqrt{2\pi r}} dr. \] (2.19)

Integrating and solving for \( r_p \) gives:

\[ r_p = 2r_y = \frac{1}{\pi} \left( \frac{K_1}{\sigma_{ys}} \right)^2. \] (2.20)

When the plastic zone size \( r_p \) is determined, the CTOD at the crack tip is given as

\[ \delta = \frac{\kappa_2 + 1}{\mu_2} K_1 \sqrt{\frac{r_{ys}}{2\pi}}. \] (2.21)

where the subscript 2 refers to the crack-embedded material. \( \kappa_2 = \frac{3-v_2}{1+v_2} \) for plane stress and \( \kappa_2 = 3 - 4v_2 \) for plane strain.
Fig. 2.10. The estimates of the plastic zone size ahead of a crack tip and the hatched area indicates elastic stress that must be redistributed by the plastic zone.

The Irwin model has been extensively used to solve the crack problems, containing the penny-shaped or arc-shaped cracks [114-118]. For example, according to the generalized Irwin model, Yi et al. [119] focused on the elastic-plastic fracture behaviors of a bi-layered plate with the consideration of a sub-interface crack. Zhuang et al. [120] studied the plastic zone correction for a sub-interface Zener-Stroh crack in a coating-substrate system. Fan et al. [121] investigated the plastic zone correction for in a bi-materials with an arbitrarily oriented Zener-Stroh crack located near their interface.

2.4.3. Plastic zone shape

It is possible to estimate the plastic zone shape of cracks by applying an appropriate yield criterion to the stress equations in Table 2.2. By substituting these equations into the von Mises yield criterion, the estimates of the Mode I plastic zone radius for the plane stress and plane strain can be obtained by
\[ r_y(\theta) = \frac{1}{4\pi} \left( \frac{K_1}{\sigma_{YS}} \right)^2 \left[ 1 + \cos \theta + \frac{3}{2} \sin^2 \theta \right], \quad (2.22a) \]

\[ r_y(\theta) = \frac{1}{4\pi} \left( \frac{K_1}{\sigma_{YS}} \right)^2 \left[ (1 - 2\nu)^2(1 + \cos \theta) + \frac{3}{2} \sin^2 \theta \right]. \quad (2.22b) \]

Then, the crack-tip plastic zone shapes for Mode I can be plotted in Fig. 2.11 (a), which describes the approximate boundary between elastic and plastic behaviors. Similarly, the estimates for Modes II and III are illustrated in Fig. 2.11 (b) and 2.11 (c), respectively. It can be seen that the extent of the plastic zone for Modes I and II in the plane strain condition is smaller than that in the plane strain state.

![Diagram of crack-tip shapes for Modes I, II, and III](image)

**Fig. 2.11.** The crack-tip shapes based on the von Mises yield criterion for different Modes of cracks.
In the 1980s, the elastic-plastic boundary for the plane stress and plane strain conditions was predicted by Banks and Garlick [122], and Cuerra et al. [123], based on the von Mises yield criterion. Subsequently, the estimates of plastic zone boundary using the Tresca criterion or small scale yielding can be used in many works [124-127]. However, all the studies mentioned above focused on the plastic zone in the isotropic materials. In the real cases, the material failure can be observed in different kinds of materials. Therefore, Khan and Khraisheh [128] studied the effect of the Hill’s anisotropic constants on the plastic shape of crack tips under the plane strain and plane stress conditions, based on the isotropic stress field and Hill’s anisotropic yield criterion. Afterwards, Gao et al. [129] combined the above criterion and small scale yielding condition to investigate the crack tip plastic zone in orthotropic materials under various loading conditions, containing pure shear loading, uniaxial loading, proportional tension shear loading, and biaxial loading. They found that the crack tip plastic zones are butterfly-like shapes and the elastic-plastic boundary is smooth in plane stress states. The crack inclination angle has significant influences on the size and shape of crack tip plastic zone. Caputo et al. [130] used the FEM to evaluate the plastic zones at crack tips influenced by the yield stress of material, the thickness of the component and the crack size.

2.5. Contact problems

The beginning of the research on the contact mechanics might be started at 1882 within the publication by Hertz. He investigated the elastic contact behavior between two elastic bodies by an analytical solution. This solution can analyze the stress distribution and deformations near the contact point. However, his study was just suitable to frictionless surface in the perfectly elastic solids. Therefore, many
researchers aimed to change these situations. A proper method to treat the frication at the contact surface would help to solve the slipping and rolling contact problems. The detailed information about the contact mechanics can be found in [131].

As a milestone in this field, Hertzian contact theory can be introduced as follow. The maximum Hertz pressure $p_0$ and the Hertz radius $a_0$ are the two basic parameters for the contact problem. When considering the three-dimensional smooth and frictionless contact problem, the expressions of two basic parameters between a half-space material and a loading sphere can be written as

$$a_0 = \left(\frac{3WR}{4\pi E'}\right)^{1/3},$$

$$p_0 = \left(\frac{6W}{\pi^{2}R^2}E'\right)^{1/3},$$

where $W$ is the external loading; $R$ is the radius of the loading sphere; and $E'$ is the effective modulus. The detailed expression for $E'$ can be obtained by

$$\frac{1}{E'} = \frac{(1 - \nu_1^2)}{E_1} + \frac{(1 - \nu_2^2)}{E_2},$$

where $E_1$ and $E_2$ are the Young’s moduli of the sphere and half-space, respectively; $\nu_1$ and $\nu_2$ are the Poisson’s ratios of the sphere and half-space, respectively. Similarly, the expressions of $a_0$ and $p_0$ for the contact problem in two-dimensional half-space can be expressed as

$$a_0 = \left(\frac{4WR}{\pi E'}\right)^{1/2},$$

$$p_0 = \left(\frac{WE'}{\pi R}\right)^{1/2}.$$

Hertz also extended his theory to provide a foundation for other contact
problems, such as load bearing capabilities, fatigue life in bearings and any other bodies where two surfaces are in contact. Afterwards, Signorini obtained a general formulation for unilateral contact problems. Recently, Johnson et al. [132] investigated the adhesive contact problems and compared their results with experiments carried out on the contact of rubber and gelatin spheres. However, this theory was rejected by Derjaguin et al. [133]. They considered the Van der Waals interactions outside the elastic contact regime and proposed the Derjaguin-Muller-Toprov (DMT) model. However, Tabor [134] proved that the Johnson-Kendall-Roberts and DMT models were two opposite extreme cases of adhesion contact condition and he could use a parameter to establish the range of applicability of the two models. Moreover, the formulation has been extensively investigated to solve the frictional contact problem [135, 136] and the elasto-plastic contact problem [137-139].

Generally, the motions of the surfaces at a contact system contain three types: sliding, rolling and spin. Sliding means the relative velocity between two surfaces is linear. When the relative angular velocity is about an axis lying in the tangent plane, it is defined as rolling motion. For the spin motion, it means that a relative angular velocity is about the common normal. These motions might induce the energy consumption and lead to material damage and structure failure. For reducing and avoiding the damage due to these motions, lubricants are usually applied to prevent the surfaces from the direct contact. Numerical works have been conducted on the EHL contact model. For example, a general EHL code was developed by Zhu and Cheng [140] to predict the coefficient of friction in the film, lubricant film thickness and flash temperature distribution on the two solid surfaces. Afterwards, Zhu and Hu [141] focused on the mixed EHL contact models, including the fluid-solid
contact and solid-solid contact coexist. A detailed review about the numerical solutions of EHL contact was conducted by Zhu and Wang [142].

Numerical studies are conducted on the EHL model with the assumption of homogeneous materials [143-145]. However, in the real cases, most components are inhomogeneous, meaning that they contain inclusions, cracks, dislocations, etc. Therefore, Dong et al. [146-151] studied the elastic properties of a half-space material or a film-substrate with multiple cracks and inhomogeneous inclusions under the EHL contact or mixed lubrication contact. They also extended this study to investigate the elastic-plastic properties of materials based on an iterative plastic loading process [152]. These works would provide guidance for reducing the material damage due to the presence of microdefects under lubricated contact.

2.6. Summary

In this chapter, the fundamentals of mechanics in the solid materials are introduced, which contain the elastic, plastic and fracture aspects. Then the different kinds of defects in materials and their modeling methods are summarized. The commonly used methods to simulate the inhomogeneous inclusions and cracks (EIM and DDT) are introduced in detail. The traditional models to investigate the crack-tip plasticity and the research based on the modified models are outlined. Finally, the basic concepts of the contact problems and their research processes are discussed.
Chapter 3 Elastic-plastic Fracture Behaviors in an Infinite Space

The interaction between the cracks and inhomogeneous inclusions in an infinite space is of significance for the material fracture behaviors. Due to the presence of microdefects, the stress distribution in the material can be changed dramatically, especially when considering the plastic zones of crack tips. In this chapter, the effect of the parameters of inhomogeneous inclusions and cracks in an infinite space on the plastic zone sizes of crack tips is studied.

3.1. Methodology

3.1.1. Problem description and solution approach

In this chapter, a two-dimensional \((xOy\) Cartesian coordinate system) problem with multiple cracks \(\Gamma_\varphi (\varphi = 1, 2, \cdots, n)\) and inhomogeneous inclusions \(\Omega_\psi (\psi = 1, 2, \cdots, m)\) with elastic moduli \(C^{\varphi}_{ijkl} (i, j, k, l = 1, 2)\) in an elastic-perfectly plastic infinite space with \(C_{ijkl}\) under external loading \(\sigma_{yy}^\infty\) is considered, as shown in Fig. 3.1 (a). The red lines ahead of cracks represent the plastic zones. Each inhomogeneous inclusion contains initial eigenstrains denoted by \(\varepsilon_{ij}^P\).

In order to deal with the governing equations for the inhomogeneous infinite space problem, cracks can be treated as a distribution of glide and climb edge dislocations with unknown densities \(\rho^+\) and \(\rho^\perp\) based on the DDT, while inhomogeneous inclusions can be simulated as homogeneous inclusions with initial eigenstrains \(\varepsilon_{ij}^P\) plus unknown equivalent eigenstrains \(\varepsilon_{ij}^*\) by means of the EIM. Then, this inhomogeneous infinite space problem can be transformed into a homogeneous problem as shown in Fig. 3.1 (b).
Fig. 3.1. The original problem of multiple cracks (a) and the new problem of multiple dislocation distributions (b) under remote stress; the red lines are the plastic zones of crack tips.

A discretization method is used to solve the governing equations for the proposed problem. This computational domain $D$, containing all the inclusions $\Omega_\psi$ ($\psi = 1, 2, \cdots m$) and cracks $\Gamma_\varphi$ ($\varphi = 1, 2, \cdots n$), is chosen as shown in Fig. 3.2. The entire domain is discretized into $N_x \times N_y$ square elements of the same size $2\Delta_x \times 2\Delta_y$. Each element can be indexed by a sequence of two integers $(\alpha, \beta)$ with $0 \leq \alpha \leq N_x - 1, 0 \leq \beta \leq N_y - 1$. In the meshed domain, provided a crack is horizontally oriented, it can be discretized into many short line segments. Each segment can be modeled as a distributed dislocation segment along the central line of the corresponding element. In each segment, the dislocation densities could be approximated by linear functions along each crack segment $\rho^+ = c^+ x + d^+$ and $\rho^\perp = c^\perp x + d^\perp$. Given a fine enough discretization, these linear functions can well approximate the practical nonlinear dislocation densities, which can be shown in Fig 3.3.
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The aims of the governing equations are to calculate the unknown equivalent
eigenstrains and dislocation densities which are used to model the inhomogeneous
inclusions and cracks, respectively. Based on the calculation results, the stress
distribution in the infinite space can be obtained. The detailed information on the
calculation of these unknowns and stress distribution in an infinite space can be
found in Appendix A.

Here, all cracks are assumed as parallel to the $x$ axis. This model can also be
applicable to vertical cracks without adding extra difficulties. Furthermore, with this
method a crack with arbitrary direction can be treated as a zigzag crack consisting
of many small vertical and horizontal crack segments.

![Discretization of the computational domain with multiple cracks and inclusions into $N_x \times N_y$ elements of the same size.](image)

Fig. 3.2. Discretization of the computational domain with multiple cracks and inclusions into $N_x \times N_y$ elements of the same size.
Fig. 3.3. A crack is modeled by a distribution of dislocations approximated by a piecewise linear function.

For sharp cracks, the stresses at crack tips can be theoretically predicted as infinite, however, it is not accurate physically since the radius of crack tips should be finite in the actual case. By introducing plastic zones ahead of crack tips, the fracture analysis of materials becomes more accurate. Based on the Dugdale model of small scale yielding, the plastic zones ahead of crack tips are one-dimensional line segments, whose size can be obtained by canceling the SIF due to the closure stress $K_{I \rho}$ and the SIF due to the applied load $K_1$ [153]:

$$K_1 + K_{I \rho} = 0. \tag{3.1}$$

It should be noted that the canceling location of the SIFs of the crack is at the tip of the plastic strip. Due to the presence of inhomogeneous inclusions, the SIFs ($K_1$ and $K_{II}$) exist simultaneously even if only the uniform tensile stress is applied. The condition to obtain the plastic zone size of cracks interacting with inhomogeneous inclusions in an infinite space can be rewritten as follows:

$$\begin{align*}
K_1^L + K_{I \rho}^L &= 0, \\
K_1^R + K_{I \rho}^R &= 0, \\
K_{II}^L + K_{I \rho}^L &= 0, \\
K_{II}^R + K_{I \rho}^R &= 0.
\end{align*} \tag{3.2}$$
where superscripts $L$ and $R$ indicate the left and right crack tips, respectively; the subscripts I and II indicate the Modes I and II cracks, respectively.

In order to solve Eq. (3.2), we need to obtain the relationship between the SIFs ($K^L_I$, $K^I_{II}$, $K^R_I$, $K^I_{II}$, $K^L_{IP}$, $K^L_{IIp}$, $K^R_{IP}$ and $K^R_{IIp}$) and the plastic zone sizes. The detailed formulas for these SIFs are introduced in Sections 3.1.2 and 3.1.3.

Due to the Dugdale model’s assumptions, the length of the plastic zone at the right tip is taken as the same as that at the left tip and the growth of plastic zones is along the direction of crack length. Thus, the proposed model can be applied in the cases in which the stress distribution around the cracks due to the disturbances of the inhomogeneous inclusions (affected by their locations and material dissimilarities) can satisfy the assumptions.

In this study, the plastic strips are also modeled by dislocations according to the DDT. Their length can be determined by cancelling the SIF due to the closure stress and that due to the applied load at the tip of the plastic strip.

### 3.1.2. Calculation for the SIFs due to the closure stress

Based on the Dugdale model, the effective crack length equals $l + \rho_R + \rho_L$, as shown in Fig. 3.4. The original crack length is set to be $l$. The plastic zone size of the right crack tip $\rho_R$ should be equal to that of the left crack tip $\rho_L$, which means that $\rho_R = \rho_L = \rho$. The interactions among the cracks and inhomogeneous inclusions in an infinite space may cause both normal and tangential tractions at the crack tips even though the space is under a simple loading condition. It also implies that the SIFs of Modes I and II ($K_I$ and $K_{II}$) should be taken into consideration for
the crack tips. Thus, $K_{I_p}$ induced by the normal closure stress $\sigma_y$ and $K_{II_p}$ caused by the shear closure stress $\tau_{xy}$ should be considered and the stresses at the crack tips should satisfy the von Mises yield criterion. The detailed distribution of the closure stresses $D(x)$ at the plastic zone can be written as

$$D_y(x) = \begin{cases} 
\sigma_y, & (-\rho_L - \frac{l}{2} < x < -\frac{l}{2} \text{ and } \frac{l}{2} < x < l + \rho_R) \\
0, & \text{(else)}
\end{cases},$$

$$D_x(x) = \begin{cases} 
\tau_{xy}, & (-\rho_L - \frac{l}{2} < x < -\frac{l}{2} \text{ and } \frac{l}{2} < x < l + \rho_R) \\
0, & \text{(else)}
\end{cases},$$

$$\sqrt{\sigma_y^2 + 3\tau_{xy}^2} = \sigma_{YS},$$

where $\sigma_{YS}$ is the yield stress of the matrix material.

Fig. 3.4. The plastic zones and yield stress distributions of a Dugdale model crack.

According to the fracture mechanics, the SIF due to the normal stress $K_{I_p}$ and that due to the shear stress $K_{II_p}$ can be given by

$$K_{I_p} = -\frac{\sigma_y}{\sqrt{\pi(a + \rho)}} \int_{a}^{a+\rho} \left\{ \frac{a + \rho + x}{a + \rho - x} + \frac{a + \rho - x}{a + \rho + x} \right\} dx$$

$$= -2\sigma_y \sqrt{\frac{a + \rho}{\pi}} \cos^{-1} \left( \frac{a}{a + \rho} \right),$$

(3.4a)
\[ K_{\Pi p} = -\frac{\tau_{xy}}{\sqrt{\pi(a + \rho)}} \int_a^{a + \rho} \left\{ \frac{a + \rho + x}{a + \rho - x} + \frac{a + \rho - x}{a + \rho + x} \right\} dx \]
\[ = -2\tau_{xy} \sqrt{\frac{a + \rho}{\pi}} \cos^{-1} \left( \frac{a}{a + \rho} \right) \] . \ (3.4b)

3.1.3. Calculation for the SIFs due to the applied load

According to the SIF definition [153], the expressions of \( K_I \) and \( K_{\Pi} \) for the crack with length \( l \) can be obtained by

\[ K_I = \lim_{x \to l} \sqrt{2\pi(x - l)} \sigma_{yy} = \frac{2\mu}{\pi(k + 1)} \lim_{x \to l} \sqrt{2\pi(x - l)} \left[ x - \xi \int_0^l \rho^+(\xi) d\xi \right] \] , \ (3.5a)

\[ K_{\Pi} = \lim_{x \to l} \sqrt{2\pi(x - l)} \sigma_{xy} = \frac{2\mu}{\pi(k + 1)} \lim_{x \to l} \sqrt{2\pi(x - l)} \left[ x - \xi \int_0^l \rho^-(\xi) d\xi \right] \] , \ (3.5b)

where \( \sigma_{yy} \) and \( \sigma_{xy} \) are the stress components due to the external loading and cracks.

Eq. (3.5) can be normalized to the interval [-1,1] by writing \( \xi = \frac{l}{2} (1 + t) \) and \( x = \frac{l}{2} (1 + s) \). Setting \( \phi^+(t) = \sqrt{1 - t^2} \rho^+(t) \) and \( \phi^-(t) = \sqrt{1 - t^2} \rho^-(t) \),

Eq. (3.5) is converted to the non-dimensional equations:

\[ K_I = \frac{2\mu}{\pi(k + 1)} \frac{1}{s \to 1} \left[ \sqrt{\pi l(s - 1)} \int_{-1}^1 \frac{\phi^+(t)}{(s - t)\sqrt{1 - t^2}} dt \right] \] , \ (3.6a)

\[ K_{\Pi} = \frac{2\mu}{\pi(k + 1)} \frac{1}{s \to 1} \left[ \sqrt{\pi l(s - 1)} \int_{-1}^1 \frac{\phi^-(t)}{(s - t)\sqrt{1 - t^2}} dt \right] \] . \ (3.6b)

Thus,

\[ K^I_L = \frac{\mu \sqrt{2\pi l}}{(k + 1)} \phi^+(1), \] \ (3.7a)

\[ K^R_L = -\frac{\mu \sqrt{2\pi l}}{(k + 1)} \phi^+(1), \] \ (3.7b)
where the superscripts $L$ and $R$ represent the left and right crack tips, respectively.

When the unknown dislocation densities $\rho^\perp$ and $\rho^\parallel$ are determined by an iterative procedure, the functions $\phi^\perp(t)$ and $\phi^\parallel(t)$ can be expressed as a polynomial of order $N$ with unknown coefficients:

$$\phi(t) = \sum_{n=0}^{N} a_n t^n. \quad (3.8)$$

These unknown coefficients $a_n$ can be determined by the data fitting using the least square method. Then, Eq. (3.7) can be written as

$$K_{II}^L = \frac{\mu\sqrt{2\pi l}}{(\kappa + 1)} \sum_{n=0}^{N} a_n^\perp, \quad (3.9a)$$

$$K_{II}^R = -\frac{\mu\sqrt{2\pi l}}{(\kappa + 1)} \sum_{n=0}^{N} (-1)^n a_n^\perp, \quad (3.9b)$$

$$K_{II}^L = \frac{\mu\sqrt{2\pi l}}{(\kappa + 1)} \sum_{n=0}^{N} a_n^\parallel, \quad (3.9c)$$

$$K_{II}^R = -\frac{\mu\sqrt{2\pi l}}{(\kappa + 1)} \sum_{n=0}^{N} (-1)^n a_n^\parallel. \quad (3.9d)$$

### 3.1.4. Numerical procedure for the entire problem

In order to solve the plastic zone sizes of cracks, we predefine the initial values, external loadings and material parameters. Then, an iterative procedure is used to obtain the plastic zone sizes until the condition Eq. (3.2) is satisfied. More
specifically, the stress distribution due to the cracks and inhomogeneous inclusions need to be obtained firstly. The results for $K_I, K_{II}, K_{I\rho}$ and $K_{II\rho}$ can be calculated according to Eqs. (3.4) and (3.9). $\rho$ decreases (increases) when $K_I < K_{I\rho}$ ($K_I > K_{I\rho}$). $\rho$ decreases (increases) when $K_{II} < K_{II\rho}$ ($K_{II} > K_{II\rho}$). This procedure is repeated until the errors (between $K_I$ and $K_{I\rho}$, $K_{II}$ and $K_{II\rho}$) are small enough. The whole flowchart for the plastic zone sizes of materials with multiple cracks and inhomogeneous inclusions in an isotropic infinite space subjected to the remote tensile loading is shown in Fig. 3.5.

![Flowchart for the plastic zone sizes of cracks interacting with inhomogeneous inclusions in an infinite space under the remote loading.](image)

**Fig. 3.5.** Flowchart for the plastic zone sizes of cracks interacting with inhomogeneous inclusions in an infinite space under the remote loading.

### 3.2. Model verification

In order to verify the proposed method to obtain the plastic zone sizes of cracks, the solution for a crack with original length $2a$ ($a$ is a fixed value) beneath an
infinite space under the uniform tension $T$ is considered. Its result is compared with the analytical solution of Dugdale. Fig. 3.6 plots the effect of the applied stress $T$ over the yield stress of matrix materials ($\sigma_{YS} = 600$ MPa) on the plastic zone size of crack tips in an infinite space under the remote tension stress. The results of the current method show a good agreement with the Dugdale analytical solution.

![Graph showing plastic zone size vs. applied stress/Yield stress](image)

**Fig. 3.6.** Comparison of the results between the Dugdale crack model and the present model.

### 3.3. Numerical results

The developed solution is used to investigate the plastic zone problems concerning the remote stress loaded in an infinite space containing two cracks, one crack and two inclusions, and two cracks and two inclusions, respectively. Since the configurations of the inhomogeneous inclusions and cracks are special in this chapter, the dislocation density distributions are anti-symmetric with respect to the crack center.
3.3.1. Plastic zones of two cracks in an infinite space

This section concerns the plastic zones of two cracks in an infinite space (Fig. 3.7) under the remote tensile stress $\sigma_{yy}^{\infty} = 360$ MPa. The matrix is assumed to be steel ($E_s = 200$ GPa, $\sigma_{YS} = 600$ MPa and $\nu_s = 0.28$); thus the plastic zones will be governed by small-scale yielding. The original length of the two cracks is $2a$. The distance between these two cracks is set to be $d = \lambda a$. According to Fig. 3.8, the SIFs at the crack tips decrease clearly with the increment of the ratio ($2a/d$) and a good agreement between the theoretical solution and the current method can be found. Therefore, an accurate prediction for the plastic zone sizes of two cracks in an infinite space can be obtained by the current model.

Fig. 3.7. Schematic of the plastic zones of two cracks in an infinite space under remote stress.
Using the same material with the verified model, the plastic zone sizes and stress distributions of an infinite space with two cracks under the remote stress $\sigma_\infty = 240$ MPa are studied. In this case, the distance between two cracks is fixed at $2.5a$, which means that $2a/d$ is equal to 0.8. The computational domain $5a \times 4a$ is meshed in $100 \times 80$ elements. The contours of the von Mises stress and other stress components in the infinite space are illustrated in Fig. 3.9. The closure stresses applied on the plastic zones can be seen apparently. The plastic zone size ahead of crack tips in this case is $0.4a$.

Fig. 3.10 presents the climb dislocation densities $\rho^\perp$ along the half effective crack length. It can be found that the dislocation density at the crack tip tends to infinite. This study is conducted under the remote tensile stress, so the glide dislocation densities $\rho^\parallel$ are much smaller than the climb dislocation densities $\rho^\perp$. 

Fig. 3.8. SIFs of the model with two cracks in an infinite space under remote stress [64].
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Fig. 3.9. The von Mises stress and other stress components distribution of two cracks in an infinite space: (a) $\sigma_{xx}$, (b) $\sigma_{yy}$, (c) $\tau_{xy}$, and (d) $\sigma_{VM}$.

Fig. 3.10. The climb dislocation density $\rho^\perp$ along the half crack length.
3.3.2. One crack and two square inclusions ahead of crack tips

Fig. 3.11 plots the schematic of an infinite space with two square inclusions ahead of one crack under the remote tensile loading \( \sigma_{yy}^{\infty} = 240 \) MPa. The original length of the crack and the side length of the inclusions are both \( 2a \). The crack \( \Gamma_1 \) is centered at \((4a,1.5a)\), and the two inclusions \( \Omega_1 \) and \( \Omega_2 \) are centered at \((1.5a,1.5a)\) and \((6.5a,1.5a)\), respectively. The matrix has the Young’s modulus \( E_s = 210 \) GPa, the Poisson’s ratio \( \nu_s = 0.28 \) and the yield stress \( \sigma_{YS} = 600 \) MPa. The two inhomogeneous inclusions have the same Young’s modulus \( E_I = 400 \) GPa and Poisson’s ratio \( \nu_I = 0.3 \). The computational domain \( 8a \times 3a \) is discretized into \( 320 \times 120 \) elements.

![Schematic diagram of an infinite space with a crack and two inclusions](image)

**Fig. 3.11.** Schematic of an isotropic infinite space with one crack interacting with two square inclusions ahead of crack tips under the remote stress.

When the plastic zones of crack tips are not taken into account, it can be found from Fig. 3.12 that the SIFs of crack tips decrease gradually with the increment of Young’s modulus of inhomogeneous inclusions. Here, \( K_0 \) is the SIF of the crack when no inclusion exists in the infinite space. It can be obtained when the Young’s
modulus of inclusions satisfies the condition $E_s = E_I$. Afterwards, the effect of the Young’s modulus of inclusions on the stress distributions and plastic zones of the crack in an infinite space is investigated. The detailed stress distribution for the case in which the Young’s modulus of inclusions equals 400 GPa is plotted in Fig. 3.13. Moreover, as the Young’s modulus of inclusions increases from 100 to 800 GPa, the ratio between the plastic zone size and the original half crack length decreases from 0.4 to 0.175 as shown in Fig. 3.14.

**Fig. 3.12.** SIFs of crack tips influenced by the Young’s modulus of inhomogeneous inclusions ahead of crack tips.
Fig. 3.13. The stress components and von Mises stress distribution in an infinite space: (a) $\sigma_{xx}$, (b) $\sigma_{yy}$, (c) $\tau_{xy}$, and (d) $\sigma_{VM}$.

Fig. 3.14. The plastic zone size of one crack interacting with two inclusions ahead of crack tips with various Young’s modulus.
Furthermore, the distributions of the climb dislocation density $\rho^\perp$ are studied due to the presence of inhomogeneous inclusions, as shown in Fig. 3.15. It is noted that the density distributions are anti-symmetric and tend to infinite at the effective crack tips. With the increment of the Young’s modulus of the inhomogeneous inclusions, the dislocation density at the effective crack tips decreases obviously.

**Fig. 3.15.** The climb dislocation densities $\rho^\perp$ along the crack length influenced by various Young’s modulus of inhomogeneous inclusions.

Moreover, the effect of the distance $d$ between the crack tip and inclusion side on the plastic zone size is also investigated. The results show that with the increment of $d$ from $0.5a$ to $1.25a$, the ratio between the plastic zone size at the crack tips and the original half crack length decreases from 0.4 to 0.275 according to Fig. 3.16. The effect of inhomogeneous inclusions on the plastic zone size of crack tips decreases dramatically with the increase of $d$ from $0.5a$ to $0.75a$ and this effect becomes increasingly weaker when the distance $d$ is larger than $1.25a$. 

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For the Dugdale model, the CTOD can be defined as the relative displacement between crack faces at the end of the strip-yield zone. Based on the DDT, it can be calculated by summing the climb and glide dislocation densities. Fig. 3.17 illustrates the CTODs in Mode I along the effective crack length for the case $E_t = 400$ GPa. It shows that they are symmetric about the crack center. The value at the original crack tip is about $9.34 \times 10^{-8}$. Compared with this value, the value of the CTOD in Mode II is much smaller due to the remote tensile loading. Therefore, the critical CTOD mainly depends on the normal CTOD. Generally, when considering the plastic strips, the CTOD has already reached the critical CTOD and induced the imminent crack extension.
Fig. 3.17. The CTODs distribution along the effective crack length.

3.3.3. Two square inclusions on both sides of one crack

Fig. 3.18 illustrates two inhomogeneous inclusions on both sides of one crack in an infinite space subjected to the remote tensile loading $\sigma_{yy}^{\infty} = 240$ MPa. The original length of the crack and the side length of the inhomogeneous inclusions are both $2a$. The crack $\Gamma_1$ is centered at $(1.5a, 2.5a)$, and the two inclusions $\Omega_1$ and $\Omega_2$ are centered at $(1.5a, 1.25a)$ and $(1.5a, 3.75a)$, respectively. The material properties of the matrix material and inclusions in this section are the same as those in section 3.3.2. The computational domain $3a \times 5a$ is discretized into $120 \times 200$ elements.
When the plastic zones of crack tips are not taken into consideration, the trend of SIFs at crack tips in this case is similar to that shown in Fig. 3.12. However, according to Fig. 3.19, it can be found that the influence of the inhomogeneous inclusions in this part is more significant than that in section 3.3.2. Moreover, Fig. 3.20 illustrates the contours of the von Mises stresses and other stress components in an infinite space with two square inhomogeneous inclusions \((E_i = 800\ \text{GPa})\) on both sides of one crack. In this case the stress concentrations can be seen more clearly. It is also found that the stresses at the corners around the inclusions in this case demonstrate weaker concentrations than that in the above case of section 3.3.2. Fig. 3.21 shows that the ratio between the plastic zone size and the original half crack length increases with the increment of Young’s modulus of inclusions on both sides of the crack. Moreover, it is also found that the effect of the distance between the crack and inclusions on the plastic zone size in this case is not very obvious.
Fig. 3.19. SIFs of crack tips influenced by the Young’s modulus of inhomogeneous inclusions on both sides of one horizontal crack.
Fig. 3.20. The stress components and von Mises stress distribution in an infinite space: (a) $\sigma_{xx}$, (b) $\sigma_{yy}$, (c) $\tau_{xy}$, and (d) $\sigma_{VM}$.

Fig. 3.21. The plastic zone size of one crack influenced by two inclusions on both sides with various Young’s modulus.
3.3.4. Two cracks and two square inclusions

Fig. 3.22 shows the schematic of an infinite space with two inhomogeneous inclusions and two cracks subjected to the remote tensile loading $\sigma_{yy}^\infty = 240$ MPa. The original length of the cracks and the side length of the inhomogeneous inclusions are both $2a$. The two cracks $\Gamma_1$ and $\Gamma_2$ are centered at $(4a, 0.5a)$ and $(4a, 2.5a)$, respectively. The two inclusions $\Omega_1$ and $\Omega_2$ are centered at $(1.5a, 1.5a)$ and $(6.5a, 1.5a)$, respectively. The material properties of the matrix and inclusions in this section are the same as those in section 3.3.2. The computational domain $8a \times 3a$ is discretized into $320 \times 120$ elements.

Fig. 3.22. Schematic of an isotropic infinite space with two cracks and two inhomogeneous inclusions subjected to the remote tension stress.

Fig. 3.23 plots the contours of the stress components and von Mises stress for the case in which all the inclusions have the same Young’s moduli $E_1 = 600$ GPa. The plastic zone size of crack tips in this case is $0.1a$. According to Fig. 3.24, it can be found that the ratio between the plastic zone size and the original half crack
length decreases from 0.275 to 0.1 with the increment of the Young’s modulus of inhomogeneous inclusions from 75 to 600 GPa.

Fig. 3.23. The stress components and von Mises stress distribution in an infinite space: (a) $\sigma_{xx}$, (b) $\sigma_{yy}$, (c) $\tau_{xy}$, and (d) $\sigma_{VM}$. 
Fig. 3.24. The plastic zone size of crack tips influenced by two inclusions with various Young’s modulus.

Moreover, the effect of the distance between two cracks on the plastic zone size is investigated. As shown in Fig 3.25, the plastic zone size reduces obviously as the distance between two cracks decreases. The effect of the distance from $a$ to $0.5a$ is larger than that from $2a$ to $a$. However, it is also found that the decrease of the SIFs at crack tips weakens obviously when this distance is smaller than $0.5a$. This phenomenon is called the shielding effect of the SIFs for two parallel cracks in close proximity to each other.
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Fig. 3.25. The plastic zone size of crack tips influenced by the distance between two cracks.

3.4. Summary

In this chapter, a semi-analytic solution is proposed to investigate the elastic-plastic fracture behaviors in an infinite space with cracks and inhomogeneous inclusions under the remote tensile stress. To obtain this solution, a combined method based on the EIM and DDT is applied.

In this study, the computational domain is discretized into many small elements with the same size. We treat the eigenstrain in each element as uniform, provided that the size of each element is small enough. Since one inhomogeneous inclusion is composed of multiple elements, the eigenstrain in any inclusion can still be non-uniform. Therefore, the effect of the shape of the inhomogeneous inclusions is considered in this study.

The current model has been validated by comparison with the theoretical
results of Dugdale. Since this study considers the influence of inhomogeneous inclusions, the Dugdale model should be modified. The effect of the Young’s moduli and positions of inhomogeneous inclusions on the plastic zone sizes of crack tips has been studied. Owing to the generality of the formulated problem, this solution has potential applications in solving a wide range of inhomogeneity-related problems.
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The cracks are usually located near the material surface subjected to the prescribed pressure or contact loading, which might make the damage effect more prominent compared with the result of cracks in an infinite space under remote stress. In this chapter, the stress distribution and plastic zone sizes of an elastic-perfectly plastic half-space with cracks under the prescribed pressure or contact loading is investigated based on the modified Dugdale model of small scale yielding.

4.1. Methodology

4.1.1. Solution for the problem under the prescribed pressure

The current problem to be solved is shown in Fig. 4.1(a), where a two-dimensional model (xOz Cartesian coordinate system) is used to study the plastic zone sizes ($\rho_L$ and $\rho_R$) and subsurface stress distributions of an elastic-perfectly plastic half-space with the crack $\Gamma$ under the prescribed loading $P$. Based on the DDT, the original two-dimensional inhomogeneous problem can be converted into a homogeneous problem as shown in Fig. 4.1(b). Since the crack is in a half-space under the external loading, $K_I$ and $K_{II}$ caused by the applied loading exist simultaneously. Therefore, the modified condition is used to solve the plastic zone sizes of cracks in a half-space. The calculation methods to obtain the SIFs due to the closure stresses and the external loading are the same as those in Chapter 3. Before this, the stress distribution in a half-space should be obtained, which will be described in the following part in detail.
(a) Calculation of the substrate stress in a half-space

The substrate stress calculation is an important step to investigate the plastic zones at crack tips. In this section, the substrate stress contains two parts: (1) the stress $\sigma_{ij}^0$ induced by the external loading and (2) the stress $\sigma_{ij}^\Gamma$ caused by cracks. Since the stresses along the cracks should satisfy the free-surface traction condition, the governing equation for the problem of cracks in a half-space can be given as

$$\sigma_{ij}^\Gamma + \sigma_{ij}^0 = 0 \ (i, j = 1, 2) \ \text{along crack } \Gamma_1. \quad (4.1)$$

In order to solve this equation, a rectangular computational domain is chosen and discretized into $N_x \times N_z$ elements with the same size $2\Delta_x \times 2\Delta_z$, as shown in Fig. 4.2. Each element can be indexed by a sequence of two integers $(\alpha, \gamma)$ with $0 \leq \alpha \leq N_x - 1, 0 \leq \gamma \leq N_z - 1$. 

Fig. 4.1. Schematic of the half-space problem with plastic zones at crack tips under prescribed loading: (a) the original problem and (b) the transformed homogeneous problem.
By using the Hooke’s law and stress superposition, the discretization expression for the stress $\sigma_{ij}^\Gamma$ at the observation point $(x_\alpha, z_\gamma)$ can be obtained according to the work done by Zhou and Wei [96]:

$$
\sigma_{\alpha\gamma}^\Gamma = \frac{2\mu}{\pi(k + 1)} \sum_{\xi=0}^{N_\zeta-1} \sum_{\zeta=0}^{N_\xi-1} \left( E_{a-\xi,y-\zeta}^\perp c^\perp_{\xi,\zeta} + F_{a-\xi,y-\zeta}^\perp d^\perp_{\xi,\zeta} + E_{a-\xi,y-\zeta}^\parallel c^\parallel_{\xi,\zeta} + F_{a-\xi,y-\zeta}^\parallel d^\parallel_{\xi,\zeta} \right) + F_{a-\xi,y-\zeta}^{d\parallel_{\xi,\zeta}} (4.2)
$$

(0 \leq \alpha \leq N_x - 1, 0 \leq \gamma \leq N_z - 1),

where $\mu$ is the shear modulus; $k$ is the Kolosov constant ($k = 3 - 4\nu$ for the plane strain problem with $\nu$ being the Poisson’s ratio); $c^\perp_{\xi,\zeta}$, $d^\perp_{\xi,\zeta}$, $c^\parallel_{\xi,\zeta}$ and $d^\parallel_{\xi,\zeta}$ are the unknown edge dislocation parameters; and $E_{a-\xi,y-\zeta}^\perp$, $F_{a-\xi,y-\zeta}^\perp$, $E_{a-\xi,y-\zeta}^\parallel$, and $F_{a-\xi,y-\zeta}^{d\parallel_{\xi,\zeta}}$ are the influence coefficients relating the stresses to the climb and glide dislocations, which can be found in Appendix B.

The stress due to the external loading $\sigma_{ij}^0$ can be obtained by integrating the constant surface pressure at the surface area. Then, the governing equation for the

Fig. 4.2. Discretization of the computational domain with cracks into $N_x \times N_z$ elements of the same size.
crack area can be given by

\[ \frac{2\mu}{\pi(\kappa + 1)} \sum_{\zeta=0}^{N_x-1} \sum_{\xi=0}^{N_x-1} \left( \mathbf{F}_{\alpha-\xi,\gamma,\zeta}^+ \mathbf{c}_{\xi,\zeta}^+ + \mathbf{F}_{\alpha-\xi,\gamma,\zeta}^- \mathbf{d}_{\xi,\zeta}^- + \mathbf{E}_{\alpha-\xi,\gamma,\zeta}^+ \mathbf{c}_{\xi,\zeta}^+ \right) \]

\[ + \mathbf{F}_{\alpha-\xi,\gamma,\zeta}^- \mathbf{d}_{\xi,\zeta}^- \right) + \sum_{\xi=0}^{N_x-1} \left( \mathbf{M}_{\alpha-\xi,\gamma} p_{\xi,0} + \mathbf{T}_{\alpha-\xi,\gamma} f_{\xi,0} \right) = 0 \]

\[(0 \leq \alpha \leq N_x - 1, 0 \leq \gamma \leq N_z - 1) \quad \text{along } \Gamma_1, \]

where \( \mathbf{M}_{\alpha-\xi,\gamma} \) and \( \mathbf{T}_{\alpha-\xi,\gamma} \) are the influence coefficients relating the normal pressure \( p_{\xi,0} \) and tangential traction \( f_{\xi,0} \) to the discretized surface area of the element \([\xi, 0]\), respectively, and their detailed expressions can be found in [96].

When the unknown dislocation densities are determined iteratively using a modified CGM, the subsurface stress \( \sigma_{\alpha,\gamma} \) can be obtained by summing the stresses due to the surface loading and cracks:

\[ \sigma_{\alpha,\gamma} = \sigma_{\alpha,\gamma}^f + \sigma_{\alpha,\gamma}^0 \]

\[ = \frac{2\mu}{\pi(\kappa + 1)} \sum_{\zeta=0}^{N_x-1} \sum_{\xi=0}^{N_x-1} \left( \mathbf{E}_{\alpha-\xi,\gamma,\zeta}^+ \mathbf{c}_{\xi,\zeta}^+ \right) \]

\[ + \mathbf{F}_{\alpha-\xi,\gamma,\zeta}^- \mathbf{d}_{\xi,\zeta}^- + \mathbf{E}_{\alpha-\xi,\gamma,\zeta}^+ \mathbf{c}_{\xi,\zeta}^+ \right) + \mathbf{F}_{\alpha-\xi,\gamma,\zeta}^- \mathbf{d}_{\xi,\zeta}^- \right) + \sum_{\xi=0}^{N_x-1} \left( \mathbf{M}_{\alpha-\xi,\gamma} p_{\xi,0} + \mathbf{T}_{\alpha-\xi,\gamma} f_{\xi,0} \right). \]

\[(4.4) \]

(b) Numerical procedure for the entire problem

An iterative procedure is used to calculate the plastic zone size of cracks in an elastic-perfectly plastic half-space. Before this procedure, we need to predefine the initial values of the plastic zone size, external loadings and properties of the
substrate and cracks. Then, determination of the substrate stress distribution and unknown dislocation densities can be obtained by using another iterative process. According to the results obtained by this process, $K_1, K_{II}, K_{I\rho}$ and $K_{II\rho}$ can be calculated by substituting the substrate stress and dislocation densities into Eqs. (3.4) and (3.9). $\rho$ decreases (increases) when $K_1 < K_{I\rho}$ ($K_1 > K_{I\rho}$). $\rho$ decreases (increases) when $K_{II} < K_{II\rho}$ ($K_{II} > K_{II\rho}$). Then, the new substrate stress distribution and unknown dislocation densities can be obtained by updating the stress distribution of the plastic zone and repeating the iterative process. Based on these new results, the SIFs are calculated and compared with those obtained in the last step. This procedure is repeated until the modified condition Eq. (3.2) to cancel out SIFs is sufficiently satisfied. Fig. 4.3 shows the whole flowchart for solving the plastic zone size of cracks in an elastic-perfectly plastic half-space under the prescribed loading.

![Flowchart for determining the sizes of the plastic zone sizes of cracks in an elastic-perfectly plastic half-space under the prescribed loading.](image)

Fig. 4.3. Flowchart for determining the sizes of the plastic zone sizes of cracks in an elastic-perfectly plastic half-space under the prescribed loading.
4.1.2. Solution for the problem under contact loading

In this section, we consider a two-dimensional ($xOz$ Cartesian coordinate system) contact problem between a rigid cylinder ($E_R$ and $v_R$) with the radius $R$ and an elastic-perfectly plastic half-space ($E_S$ and $v_S$) with cracks $\Gamma_\varphi (\varphi = 1,2,\cdots m)$, as shown in Fig. 4.4(a). The contact problem is induced by the normal load $W$ pushing the cylinder into the half-space material. The red lines ahead of crack tips are the plastic zones according to the Dugdale model. Based on the DDT, the original contact problem (Fig. 4.4(a)) in an inhomogeneous elastic-perfectly plastic half-space can be transformed into a homogeneous contact problem (Fig. 4.4(b)).

**Fig. 4.4.** Schematic of the contact system with the plastic zones (red lines) of the cracks: (a) the original problem and (b) the converted homogeneous problem.

**Two-dimensional half-space homogeneous contact problem**

This two-dimensional contact problem uses the same discretization method as that in section 4.1.1. In the computational domain, a half-space subjected to the cylindrical contact loading can be solved by the following equations and inequalities:
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\[ W = \sum_{\alpha=0}^{N_x-1} 2\Delta_x p_{\alpha,0}, \]  
(4.5a)

\[ h_\alpha = h^i_\alpha + \sum_{\xi=0}^{N_x-1} (Q^n_{\alpha-\xi} - \mu Q^f_{\alpha-\xi}) p_{\xi,0} - \delta, \]  
(4.5b)

\[ p_{\alpha,0} > 0, h_\alpha = 0, \text{ in } A_c, \]  
(4.5c)

\[ p_{\alpha,0} = 0, h_\alpha > 0, \text{ outside } A_c. \]  
(4.5d)

where \( p_{\alpha,0} \) denotes the surface pressure on the element \([\alpha, 0] \); \( h_\alpha \) represents the gap between the two contact surfaces; \( h^i_\alpha \) represents the initial gap; \( Q^n_{\alpha-\xi} \) and \( Q^f_{\alpha-\xi} \) are the coefficients relating the surface displacement to the normal pressure and tangential friction, respectively; \( \delta \) represents the relative rigid body approach; \( \mu \) is the friction coefficient; and the contact area is denoted by the symbol \( A_c \).

The unknown surface pressure distribution and contact area can be obtained iteratively by a modified CGM when the surface displacement due to contact loading and the substrate cracks converges. After this, the SIFs due to the closure stress and the external loading can be obtained.

**Numerical procedure for the entire problem**

In order to solve the plastic zone size and subsurface stress distribution of materials with cracks, we redefine the initial values for the plastic zone size, parameters of the half-space and loading body, and the external loadings. Then, an iterative procedure is applied to ensure that the condition Eq. (3.2) is satisfied. Before the results of \( K_1, K_{II}, K_{IIP} \) and \( K_{III} \) are calculated according to Eqs. (3.4) and (3.9), the iterative process to obtain the surface displacement due to the substrate cracks and contact loading must be done firstly until this displacement
converges by a numerical algorithm. The detailed calculation method for this surface displacement can be found in Appendix C. \( \rho \) decreases (increases) when \( K_1 < K_{1p} \) (\( K_1 > K_{1p} \)). \( \rho \) decreases (increases) when \( K_{II} < K_{IIp} \) (\( K_{II} > K_{IIp} \)). At every step of changing \( \rho \), the stresses at the effective crack length should be updated. The procedure to obtain the plastic zone size of crack tips is repeated until the errors (between \( K_1 \) and \( K_{1p} \), \( K_{II} \) and \( K_{IIp} \)) are small enough. Fig. 4.5 shows the whole flowchart for solving the plastic zone size and stress distribution of a half-space with the cracks under contact loading.

![Flowchart for the plastic zone sizes and stress distribution of cracks in an elastic-perfectly plastic half-space under contact loading.](image-url)

Fig. 4.5. Flowchart for the plastic zone sizes and stress distribution of cracks in an elastic-perfectly plastic half-space under contact loading.
Due to the limitations of the Dugdale crack model (the plastic zone of crack tips must be symmetric), the study in this chapter just considers the case that the center of the crack is along the applied loading direction, which means the plastic zone of crack tips under this condition is symmetric.

4.2. Numerical results and discussions

4.2.1. Results under the prescribed pressure

In this part, we consider a crack near an elastic-perfectly plastic half-space surface subjected to the prescribed loading $P$, as shown in Fig. 4.6. The material properties of the half-space are the Young’s modulus $E_s = 210$ GPa, the Poisson’s ratio $\nu_s = 0.28$ and the yield stress $\sigma_{YS} = 550$ MPa. The external loading is set to be $P=175$ MPa. The length and depth of the crack are set as $l = 2a$ ($a$ is a fixed value) along the $x$-axis and $h = 2a$ along the $z$-axis, respectively. The plastic zone size ahead of the crack tips is set to be $\rho$.

![Fig. 4.6. Schematic of one horizontal crack and its plastic zones in an elastic-perfectly plastic half-space under the prescribed loading.](image)

When the plastic zones of crack tips are taken into consideration, the contours of the stress components and von Mises stress distribution are illustrated in Fig. 4.7. It can be seen that the stress distribution is significantly influenced by the presence
of the crack and stress concentrations are found around the plastic zones. The plastic zone size at this condition equals 0.3a.

Fig. 4.7. Contours of the stress components and von Mises stress distribution for the crack in an elastic-perfectly plastic half-space under the prescribed loading.

**Effect of the yield stress of the matrix material**

Fig. 4.8 shows the change of the plastic zone size at crack tips with the increment of the yield stress of the matrix material. It is obvious that with the increment of the yield stress over the applied load from 2.68 to 4.85 ($\sigma_{YS} = 470$–850 MPa), the ratio between the plastic zone size of cracks tips and the original half crack length decreases from about 0.6 to 0.1. In addition, it can also be seen that the plastic zone size of crack tips changes significantly when the yield stress of
the matrix material is less than 550 MPa. It can be predicted that the crack is
difficult to be closed when the yield stress of materials is too small. Moreover, with
the increment of the yield stress, the plastic zone size of crack tips will disappear.

![Graph showing plastic zone size vs. yield stress](image)

**Fig. 4.8.** The plastic zone size of a crack in an elastic-perfectly plastic half-space with various yield stresses.

**Effect of the original crack length**

Fig. 4.9 plots the change of the plastic zone size at crack tips with the increment
of the original crack length. It is found that the ratio between the plastic zone size of
 crack tips and the original half crack length increases from about 0.1 to 0.6 as the
original crack length increases from 1.2a to 2.4a. This effect becomes more
obvious when the original crack length is larger than 2a. It also indicates that the
plastic zone size of crack tips increases significantly when the original crack length
is too large.
Fig. 4.9. The plastic zone size of a crack in an elastic-perfectly plastic half-space with various crack lengths.

*Effect of the crack depth*

Fig. 4.10 shows the change of the plastic zone size at crack tips with the increment of the crack depth. It can be found that the ratio between the plastic zone size and the original half crack length increases as the crack depth decreases. This effect enhances dramatically when the crack is close to the half-space surface. For example, the ratio increases from 0.3 to 0.5 when the crack depth decreases from 2a to 1.5a. However, when the crack depth decreases from 4.5a to 2a, the ratio just increases from 0.1 to 0.3. This effect also indicates that the crack is more difficult to be closed when the crack is close enough to the surface. It can also be predicted that the depth effect on the plastic zone size of crack tips will disappear as the depth increases.
Fig. 4.10. The plastic zone size of a crack in an elastic-perfectly plastic half-space with various crack depths.

**Effect of the external loading**

This part concerns the effect of the external loading on the plastic zone size of crack tips. Fig. 4.11 shows that the plastic zone size of crack tips increases dramatically with the increment of the external loading, especially when the external loading exceeds 200 MPa. It means that with the increment of the external loading, the crack is more and more difficult to be closed. The crack will propagate and cause the fracture of materials when the external loading is too large.
4.2.2. Results under contact loading

In this section, an elastic-perfectly plastic half-space with a crack subjected to the cylindrical contact loading $W$ is taken into consideration, as shown in Fig. 4.12. The material properties of the half-space are the Young’s modulus $E_s = 210$ GPa, the Poisson’s ratio $\nu_s = 0.28$ and the yield stress $\sigma_{YS} = 450$ MPa. The cylindrical indenter has radius $R = 0.0001$ mm and is assumed to be rigid. The external loading is set to be $W = 1.0 \times 10^6$ N. The length and depth of the crack are set to be $l = 2a$ (a is a fixed value and approximate to the Hertz radius) along the x-axis and $h = 2a$ along the z-axis, respectively. The plastic zone size ahead of the crack is represented by $\rho$. The two-dimensional computational domain $8a \times 8a$ is discretized into $80 \times 80$ elements in this section.
Fig. 4.12. Schematic of a crack and its plastic zones in a half-space under contact loading.

In this numerical example, the plastic zone sizes of crack tips and their influences on the substrate stress distribution of materials are studied. Fig. 4.13 shows that the plastic zone size over the original half crack length at this condition is 0.5. The maximum von Mises stress decreases from 950 to 900 MPa after taking the plastic zones of crack tips into consideration. It can be found that the stress concentrations mainly occur at the crack tips and the contact area. The stress distribution and the surface pressure distribution are significantly influenced by the plastic zones. Therefore, taking the plastic zones into consideration is beneficial to the fracture mechanics analysis and a more accurate description of the substrate stress field and the pressure distribution can be obtained. The contours of the stress components ($\sigma_{xx}$, $\sigma_{zz}$ and $\tau_{xz}$) when considering the plastic zones are plotted in Fig. 4.14.
Fig. 4.13. Comparison of the von Mises stress distribution for the crack in a half-space under contact loading: (a) considering the plastic zones of crack tips and (b) without considering the plastic zones.

Fig. 4.14. The contours of stress components ($\sigma_{xx}$, $\sigma_{zz}$ and $\tau_{xz}$) for the crack in a half-space under contact loading when considering the effect of plastic zones.

**Effect of the yield stress of the matrix material**

Fig. 4.15 shows the change of the plastic zone sizes at crack tips with the increment of the yield stress of the matrix material, i.e., $\sigma_{YS} = 350, 400, 500, 600$ and $700$ MPa. It is obvious that with the increment of the yield stress from 400 to 700 MPa, the ratio between the plastic zone size of cracks tips and the original half crack length decreases from 0.6 to 0.1. In addition, it can also be seen that when the yield stress of the matrix material is less than 400 MPa, the plastic zone size of crack tips changes dramatically. It can be predicted that the crack would be difficult
to be closed when the yield stress of the matrix material is too small. Moreover, it is obvious that the plastic zone size would be very small as the yield stress of materials increases.

**Fig. 4.15.** The plastic zone size ahead of crack tips in a half-space with various yield stresses.

*Effect of the original crack length*

Fig. 4.16 shows the change of the plastic zone size at crack tips with the increment of the original crack length. According to this figure, it is found that the ratio between the plastic zone size of crack tips and the original crack length increases from 0.1 to 0.7 as the original crack length increases from $a$ to $2.8a$. In addition, the growth rate induced by the original crack length is more smooth than that induced by other parameters, such as the yield stress, loading conditions and the crack depth. This also means that the effect of the crack length on the plastic zone size is very slight.
Fig. 4.16. The plastic zone size ahead of crack tips with various original crack lengths.

**Effect of the crack depth**

Fig. 4.17 shows the change of the plastic zone size at crack tips with the increment of the crack depth. In order to make the effect of the original crack depth clearer, the yield stress of the matrix material in this part is set to be 600 MPa and other parameters are the same as those of the previous simulation. It is obvious that the ratio between the plastic zone size and the original half crack length increases as the crack depth decreases. This effect enhances dramatically when the crack depth is close enough to the contact surface. For example, the ratio increases from 0.5 to 0.8 when the crack depth decreases from 1.5\(a\) to 1.4\(a\). However, when the crack depth decreases from 2.5\(a\) to 1.5\(a\), the ratio just increases from 0.1 to 0.5. It also indicates that the crack is more difficult to be closed when the crack is close enough to the contact surface. It could be predicted that the depth effect on the plastic zone size of crack tips will disappear as the crack depth increases.
Fig. 4.17. The plastic zone size ahead of crack tips with various crack depths.

Effect of the external loading

This part concerns the effect of the external loading conditions on the plastic zone sizes of crack tips. In this part, the yield stress of the matrix material is also set to be 600 MPa. Fig. 4.18 shows that with the increment of the external loading, the plastic zone size of crack tips changes dramatically, especially when the external loading exceeds $1.6 \times 10^{-6}$ N. It also indicates that with the increment of the external loading the crack is more difficult to be closed. It could be predicted that the crack would propagate and cause the fracture of the matrix material when the external loading is too large.
4.3. Summary

In this chapter, two semi-analytic solutions are developed for the elastic-plastic fracture behaviors of a half-space with cracks under the prescribed pressure and contact loading, respectively. The unknown surface pressure and contact area can be obtained iteratively by a modified CGM. A group of numerical examples are conducted to investigate the effect of the yield stress of the matrix material, the original length and the crack depth on the plastic zone size of crack tips in a half-space subjected to the prescribed pressure and contact loading. It can be found that the plastic zone sizes are affected significantly by the original crack length and depth, the yield strength of substrate and loading conditions. With the correction of the plastic zone sizes of crack tips, a more accurate stress distribution of a half-space with cracks under the prescribed pressure and contact loading can be obtained.
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According to the setting of the contact model, the results of contact loading would not be obtained from the prescribed pressure cases. This is because the contact area is much smaller than the subsurface crack geometry even though the contact radius is sufficiently large.

When the general solution for the elastic-plastic fracture behaviors of a half-space with microdefects under contact loading is obtained, it would have a remarkable application in addressing significant but complicated engineering problems of materials concerning the plastic deformation and the material dissimilarity.
Chapter 5 Elastic-plastic Model of a Film-substrate with Inhomogeneous Inclusions

Surface coatings have been extensively used in many mechanical components, such as cutting tools, engines and transmissions. They can protect the matrix material from the thermal or corrosive degradation and impart wear resistance to the surface. However, due to the difference between the coating and the substrate in material properties, the elastic-plastic properties of the film-substrate can be influenced significantly, especially when the contact loading is applied and microdefects are near the contact surface. Therefore, this chapter investigates the elastic-plastic behaviors of a film-substrate with inhomogeneous inclusions subjected to contact loading.

5.1. Methodology

5.1.1. Problem description and solution approach

In this chapter, we consider the contact system of a sphere \((E_R, \nu_R)\) and a film-substrate \((E_c, \nu_c, E_s \text{ and } \nu_s)\) with inhomogeneous inclusions \((E_i, \nu_i)\), as shown in Fig. 5.1(a). The external loading \(W\) is applied to the half-space surface by a rigid sphere with the radius \(R\). The half-space contains \(n\) arbitrarily-shaped inhomogeneous inclusions \(\Omega_\psi (\psi = 1,2,\cdots n)\). The elastic moduli of the matrix material, the coating material and inhomogeneous inclusions are denoted by \(C_{ijkl}\), \(C_{ijkl}^c\) and \(C_{ijkl}^\psi (i,j,k,l = 1,2,3)\), respectively.

The film-substrate contact problem with inhomogeneous inclusions can be transformed into a homogenous half-space problem as shown in Fig. 5.1(b), using the EIM.
The film is assumed to be perfectly bonded to the substrate without interface slipping and locally detaching. This film can be treated as an inhomogeneity with respect to the substrate only when two conditions are satisfied. The first one is that the length and width of the inhomogeneity are much larger than its thickness. The other one is that the width and length are much larger than the dimensions of the contact area on its surface.

The computational domain $D$ is discretized into $N_x \times N_y \times N_z$ cuboidal elements of the same size $2\Delta x \times 2\Delta y \times 2\Delta z$, as shown in Fig. 5.2. Each element can be indexed by a sequence of three integers $[\alpha, \beta, \gamma]$ with $0 \leq \alpha \leq N_x - 1$, $0 \leq \beta \leq N_y - 1$ and $0 \leq \gamma \leq N_z - 1$, and the coating material and inclusions can be approximated by a collection of these small cuboidal elements. Generally, the eigenstrains can be regarded as uniform in each cuboidal element. However, the eigenstrain in any inhomogeneous inclusion that contains multiple cuboidal
elements can still be non-uniform.

Fig. 5.2. Discretization of the computational domain with \( \psi \) inhomogeneous inclusions under the coating material into \( N_x \times N_y \times N_z \) cuboids of the same size.

Based on the work done by Zhou et al. [14] about the elastic behaviors of a half-space with multiple inclusions under contact loading, the governing equations to solve the inhomogeneous contact problem when considering the plastic behaviors can be written as

\[
(C_{ijkl}^{-1}C^{-1}_{klmn} - 1)\sigma_{ij}^* + C_{ijkl}^{\psi}(\varepsilon_{kl}^* + \varepsilon_{kl}^{**}) = (1 - C_{ijkl}^{\psi}C^{-1}_{klmq})(\sigma_{ij}^p + \sigma_{ij}^0).
\]

(5.1)

where \( \sigma_{ij}^p \) and \( \sigma_{ij}^* \) are the eigenstresses induced by the initial eigenstrain and equivalent eigenstrain in all the inclusions \( \Omega_\psi \); \( \sigma_{ij}^0 \) is the stress applied by the external loading; \( C_{ijkl}^{\psi} \) and \( C_{ijkl} \) are the elastic moduli of the inhomogeneous inclusion \( \Omega_\psi \) and the substrate, respectively; \( \varepsilon_{ij}^* \) is the equivalent eigenstrain; and \( \varepsilon_{ij}^{**} \) is the equivalent plastic strain.
In Eq. (5.1), the equivalent eigenstrain \( \varepsilon_{ij}^* \) and the equivalent plastic strain \( \varepsilon_{ij}^{**} \) are unknowns. In order to obtain these unknown strains, the unknown contact area and surface pressure distributions need to be determined firstly by an iterative process when the surface displacement induced by the contact loading, the inhomogeneous inclusions, the coating material and the effective plastic strains converge. The detailed calculation method for the contact problem of a film-substrate with inclusions will be introduced in the following sections.

### 5.1.2. Contact problem for a film-substrate with inhomogeneous inclusions

For a dry contact, the unknown surface pressure distribution and contact area can be obtained when the surface displacement converges. When considering the contact problem for a film-substrate with inhomogeneous inclusions, the surface displacement \( u(x, y) \) can be decomposed into three parts: (1) the elastic displacement induced by the surface pressure, (2) the eigen-displacement caused by the equivalent eigenstrains \( \varepsilon_{\xi,\zeta,\varphi}^* \) and the initial eigenstrains \( \varepsilon_{\xi,\zeta,\varphi}^P \), and (3) the displacement induced by the equivalent plastic strain \( \varepsilon_{\xi,\zeta,\varphi}^{**} \). Therefore, the surface displacement expression can be written as

\[
\begin{align*}
\quad u(x, y) &= \sum_{\zeta=0}^{N_x-1} \sum_{\varphi=0}^{N_y-1} Q^p_{\alpha-\xi,\beta-\zeta,\gamma} p_{\xi,\zeta} + \sum_{\zeta=0}^{N_x-1} \sum_{\varphi=0}^{N_y-1} Q^f_{\alpha-\xi,\beta-\zeta,\gamma} f_{\xi,\zeta} \\
&\quad + \sum_{\varphi=0}^{N_z-1} \sum_{\zeta=0}^{N_y-1} \sum_{\xi=0}^{N_x-1} S_{\xi-\alpha,\zeta-\beta,\varphi} (\varepsilon_{\xi,\zeta,\varphi}^P + \varepsilon_{\xi,\zeta,\varphi}^* + \varepsilon_{\xi,\zeta,\varphi}^{**})
\end{align*}
\]

(5.2)

where \( Q^p_{\alpha-\xi,\beta-\zeta,\gamma} \) and \( Q^f_{\alpha-\xi,\beta-\zeta,\gamma} \) are the influence coefficients induced by \( p_{\xi,\zeta} \) and \( f_{\xi,\zeta} \) on a surface element, respectively; and \( S_{\xi-\alpha,\zeta-\beta,\varphi} \) are the coefficients
relating the surface displacement to the initial eigenstrain $\varepsilon_{\zeta, \phi}^P$, the equivalent eigenstrain $\varepsilon_{\zeta, \phi}^t$ and the effective equivalent plastic strain $\varepsilon_{\zeta, \phi}^{t*}$, and the detailed expressions of $S_{\alpha - \zeta - \beta, \phi}$, $Q_\alpha^{n}$, $Q_\beta^{f}$, and $Q_\gamma^{f}$ can be found in the work [14].

The contact area and surface pressure distribution can be influenced by the presence of inhomogeneous inclusions and the coating material. With the initial inputs, an iterative process is used to calculate the accurate description of surface pressure and the subsurface stress distributions. The detailed calculation method for the subsurface stress field can be found in Appendix D. This process will continue until the surface displacement due to the inclusions, the coating material, the contact body and the effective plastic strain converges. In this study, the residual stresses caused by the effective plastic strains are taken into consideration. They are calculated based on the original work of Jacq et al. [4] about the eigenstresses induced by the effective plastic strains.

5.1.3. Plasticity consideration

Plasticity is an irreversible process in response to the loading conditions. Usually, the von Mises yield criterion and the Tresca yield criterion are used to identify the transition from elastic to plastic deformation. In this study, the former criterion is chosen and its detailed expression can be written as

$$f = \sigma_{VM} - g(p), \quad \text{(5.3)}$$

In Eq. (5.3), the von Mises stress is written as $\sigma_{VM} = \sqrt{3S_{ij}S_{ij}}/2$, where $S_{ij}$ is the deviatoric stress, $p$ is the accumulative plastic strain, and $g(p)$ is the yield stress related to the isotropic hardening effect. The plastic strain increment is determined
by the plastic flow rule \( \text{d}\varepsilon_{ij} = \frac{\text{d}\lambda}{\text{d}f} \frac{3S_{ij}}{2\sigma_{VM}} \), where \( \text{d}\lambda \) represents the plastic multiplier. The increment of the accumulative plastic strain is defined as \( \text{d}p = \sqrt{\frac{3}{2}\text{d}\varepsilon_{ij}^p} \), which equals \( \text{d}\lambda \). The detailed information for the calculation of the plastic strain increment can be found in Appendix E.

5.1.4. Numerical scheme

According to the governing equations for the film-substrate with inhomogeneous inclusion under contact loading, the effective plastic strain is added into the total strain when the stress of any point exceeds the yield strength of the corresponding material. Since the contact loading is applied to the surface uniformly step by step, the pressure distribution at every loading step can be obtained by a single-loop CGM. Then the subsurface stress field can be determined. The plastic domain can be identified based on the \( J-2 \) criterion. The actual increment of the effective plastic strain \( \text{d}\lambda \) is the value that returns the \( J-2 \) yield function to zero. This value can be determined by the Newton-Raphson method. Then, the plastic strain increments \( \text{d}\varepsilon_{ij}^p \) can be obtained according to the flow rule.

When the equivalent eigenstrains and eigenstresses in a film-substrate are obtained, the surface eigen-displacement can be calculated. It can influence the surface geometry and the contact pressure distribution in return. Therefore, the surface geometry is changed and the contact pressure distribution is updated again by solving a set of contact equations. A closed-loop is formed among the surface geometry, the effective plastic strain, and the contact pressure. This loop will not be ended until the difference of the eigen-displacements between the two iterative steps is less than the prescribed error tolerance. When this displacement converges, the
normal load is increased and the next load step starts. Fig. 5.3 shows the flowchart of the elastic-plastic problem of a film-substrate with inhomogeneous inclusions under contact loading.

![Flowchart](image)

**Fig. 5.3.** Flowchart for the elastic-plastic problem of a film-substrate with inhomogeneous inclusions under contact loading.

### 5.2. Model verification

Wang et al. [154] investigated the contact problem between a rigid half-space plane and an elasto-plastic sphere by the FEM. Their results are used to verify the current proposed model. The linear hardening law is employed to analyze the plastic behaviors of materials as shown in Fig. 5.4. Its Young’s modulus and initial yield stress are denoted by $E_s$ and $\sigma_Y$, respectively. The variable $E_t$ is the tangential
modulus for the linear hardening law. When it equals zero, the material
demonstrates elastic-perfectly plastic behavior. In order to keep consistent with the
work in [154], the basic properties of the half-space are the Young’s modulus
$E = 100$ GPa, the Poisson’ ratio $\nu = 0.3$ and the yield stress $\sigma_Y = 600$ MPa.
The radius of the rigid contact body $R$ is equal to 20 mm. The normal contact
loading is set to be $W = 800$ N, which can be applied averagely by 10 steps. The
surface contact pressure and dimension are normalized by the maximum Hertzian
pressure $p_0 = 1671.92$ MPa and the Hertzian radius $a_0 = 0.47798$ mm,
respectively. The computational area is defined in the dimensions $-2a_0 \leq x \leq 2a_0$,$-2a_0 \leq y \leq 2a_0$ and $0 \leq z \leq 2a_0$ with $64 \times 64 \times 32$ unit grids.

In this study, an increasing loading process is used to simulate the plastic
deformation of materials with inhomogeneous inclusions. The entire loading
process is divided into $N$ quasi-static steps. Each constant loading step $W_c$ can be
expressed as

$$W_c = \frac{(1.6\pi \sigma_Y)^3}{6} \left(\frac{R}{E'}\right)^2, \quad (5.4)$$

where $E'$ is the equivalent Young’s modulus for the homogeneous contact problem.

The distributions of contact pressures, von Mises stresses and equivalent
plastic strains with varied tangential modulus $E_t$ are plotted in Fig. 5.5 (a), (b) and
(c), respectively. It can be noted that the results from the current solution and the
FEM match very well.
Chapter 5 Elastic-plastic Model of a Film-substrate with Inclusions

Fig. 5.4. Linear hardening law ($E_t$ is the tangential modulus).
In order to verify the film-substrate model, the thickness of the coating is set to be $a_0$ and other parameters of the matrix material and loading body are the same as
those in the above model. Its results are compared with those of the O’Sullivan and king’s analytic solution [155], as shown in Fig. 5.6. Fig. 5.6(a) shows the normal surface pressure for coating materials with various elastic constants, and Fig. 5.6 (b) represents the shear stress component at the interface between the coating layer and the substrate. The results between these two methods show a good agreement.

The FEM has been extensively used to solve the elastic-plastic problems in the homogeneous space. However, when a film-substrate system with multiple microdefects under contact loading is taken into consideration, a larger number of elements are needed to mesh the entire body. This will make the numerical simulations time-consuming. In this study, the coating and inhomogeneous inclusions are decomposed into many small elements at the beginning. Therefore, the current method can treat multiple inhomogeneous inclusions and the coating material in the way as it treats one single inclusion without adding any computational complexity. Moreover, an FFT algorithm is also applied to improve the computational efficiency.
Fig. 5.6. Model validation with the O’ Sullivan and King’s solution: (a) normal pressure and (b) shear stress at the interface between the coating and the substrate.

### 5.3. Numerical results

Three-dimensional simulations are conducted using the current model for the elastic-plastic behaviors of a film-substrate with inhomogeneous inclusions involving a half-space and a punch. The punch is set to be a rigid sphere with a radius of \( R = 8 \) mm. The half-space matrix is set to be steel with the Young’s modulus \( E_s = 200 \) GPa, the Poisson’ ratio \( \nu_s = 0.3 \) and the yield stress \( \sigma_Y = 600 \) MPa. The inhomogeneous inclusions are set to have \( E_i = \gamma E_s \) and \( \nu_i = \nu_s \). The parameter \( \gamma \) indicates the material difference between the inhomogeneity and the matrix material. When \( \gamma > 1 \), the inhomogeneity is stiff compared with the matrix material, while it is compliant when \( \gamma < 1 \). The yield stress of the inhomogeneous inclusion is set to be \( \sigma_{Yi} \). The thickness of the coating material is \( d \). Its Young’s modulus and yield stress can be denoted as \( E_C \) and \( \sigma_{YC} \), respectively.
In this study, the substrate, the coating and inclusions are all elastic-perfectly plastic materials. The normal contact loading is set to be $W = 6 W_c$. The Hertzian peak pressure $p_0 = 1761.44 \text{ GPa}$ and the Hertzian radius $a_0 = 0.1007 \text{ mm}$ for homogeneous contacts are used to normalize the obtained results. The computational area is defined in the dimensions $-2a_0 \leq x \leq 2a_0, -2a_0 \leq y \leq 2a_0$ and $0 \leq x \leq 2a_0$ with $64 \times 64 \times 32$ unit grids.

### 5.3.1. One inclusion in the film-substrate

In this part, the elastic-plastic behaviors of the film-substrate with one inhomogeneous inclusion are studied as shown in Fig. 5.7. The inhomogeneous cuboids inclusion has the side length $0.5a_0$, located at $h = 0.375a_0$ and has the Young’s modulus $E_i = 400 \text{ GPa}$. Its yield stress is set to be $\sigma_{yi} = 900 \text{ MPa}$. The Young’s modulus and the yield stress of the coating material are set to be $E_c = 400 \text{ GPa}$ and $\sigma_{yc} = 600 \text{ MPa}$, respectively. Its thickness is set to be $d = 0.25a_0$. The effect of different parameters of the inclusion and the coating material on the surface pressure and stress distributions is investigated.

**Fig. 5.7.** Schematic of a film-substrate with one inhomogeneous inclusion under contact loading.
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The effect of the Young’s modulus of the inclusion on the pressure distribution is plotted in Fig. 5.8. It shows that when the film-substrate does not contain the inclusion, the surface pressure has a relatively flat profile. If one inhomogeneous inclusion in the substrate is considered, it can be found that the central peak pressure decreases with the increase of the Young’s modulus of the stiff inclusion. When the inclusion is compliant, the surface pressure decreases compared with the case without inclusion and two low points can be found at the edges of the inclusion. Figs. 5.9 and 5.10 illustrate the effect of the embedded inhomogeneous inclusion with various Young’s moduli on the von Mises stresses and effective plastic strains distributions, respectively. The maximum effective plastic strain and von Mises stress are outside the inclusion when $E_i = 0.5 E_s$, while they are inside the inclusion when $E_i = 2.5 E_s$. Moreover, it is clearly that stress concentrations mainly appear at the corners of the inclusion. Due to the presence of these concentrations, the stress distribution of the coating has been affected significantly, especially in the stiff inclusion case.

![Graph showing the effect of Young's modulus on pressure distribution](image)

**Fig. 5.8.** The effect of the Young’s modulus of inhomogeneous inclusion on the normal pressure in the central plane $y = 0$ ($E_i = 100, 200, 300, 400, 500$ GPa).
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Fig. 5.9. The effect of a compliant inhomogeneous inclusion \((E_i = 100 \text{ GPa})\) on the profiles of the (a) dimensionless von Mises stresses and (b) effective plastic strains on the \(x-z\) plane.

Fig. 5.10. The effect of a stiffer inhomogeneous inclusion \((E_i = 500 \text{ GPa})\) on the profiles of the (a) dimensionless von Mises stresses and (b) effective plastic strains on the \(x-z\) plane.

The depth influence of the inhomogeneous inclusion on the stress field and the pressure distribution is also studied in this section. Fig. 5.11 presents the surface normal pressure at a frictionless surface for various depths at which the inhomogeneous inclusion locates. It can be found that the position of the inclusion significantly affects the contact pressure distribution when it is close to the interface between the coating and the substrate. It can also be found that the central peak pressure value grows from about \(0.6 p_0\), \(0.636 p_0\) to \(0.667 p_0\) when the depth increases from \(0.375 a_0\), \(0.5 a_0\) to \(0.75 a_0\).
Fig. 5.11. The effect of the depth of inhomogeneous inclusion on the normal pressure in the central plane \( y = 0 \).

Figs 5.12 and 5.13 demonstrate the depth effect of the inhomogeneous inclusion on the effective plastic strain and von Mises stresses in the central plane \( y = 0 \) for \( h = 0.375 \, a_0 \) and \( h = 0.75 \, a_0 \), respectively. For the case with \( h = 0.375 \, a_0 \), the maximum effective plastic strain is inside the inclusion. While it occurs at the substrate above the inclusion for the case with \( h = 0.75 \, a_0 \). Moreover, the effective plastic strain increases from 0.45 to 0.55 as the depth of the inclusions decreases from \( 0.75 \, a_0 \) to \( 0.375 \, a_0 \).

Fig. 5.12. The effect of a compliant inhomogeneous inclusion \((E_i = 400 \, \text{GPa})\) of \( h = 0.375 \, a_0 \) on the profiles of the (a) dimensionless von Mises stresses and (b) effective plastic strains on the \( x-z \) plane.
Fig. 5.13. The effect of a compliant inhomogeneous inclusion \((E_i = 400 \text{ GPa})\) of \(h = 0.75 \ a_0\) on the profiles of the (a) dimensionless von Mises stresses and (b) effective plastic strains on the \(x\)-\(z\) plane.

Fig. 5.14 presents the effect of various Young’s moduli of the coating material (i.e., \(E_c/E_s = 0.5, 1.5, 2.0\) and 2.5) on the surface pressure distribution. It indicates that the influence of the Young’s modulus on the surface pressure distribution is not very obvious. Moreover, it can also be found that the surface pressure profile of the case \(E_c = 500 \text{ GPa}\) is more complex than other cases. Figs. 5.16 and 5.17 demonstrate the von Mises stress and effective plastic strain distributions for the cases \(E_c = 100 \text{ GPa}\) and \(E_c = 500 \text{ GPa}\), respectively.

Fig. 5.14. The effect of the Young’s modulus of coating material on the normal pressure in the central plane \(y = 0\) \((E_C = 100, 300, 400, 500 \text{ GPa})\).
The effect of the thickness of the coating material on the surface pressure distribution is also studied. The simulation results for the cases of $d = 0.1875a_0$, $d = 0.25a_0$ and $d = 0.3125a_0$ are shown in Fig. 5.17. It can be found that the central pressure value decreases with the increase of the thickness of the coating material. Moreover, the whole pressure profile becomes more complicated when the thickness of the coating material equals $0.3125a_0$. 

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**Fig. 5.15.** The effect of a compliant coating material ($E_C = 100$ GPa) on the profiles of the (a) dimensionless von Mises stresses and (b) effective plastic strains on the $x$-$z$ plane.

**Fig. 5.16.** The effect of a stiff coating material ($E_C = 500$ GPa) on the profiles of the (a) dimensionless von Mises stresses and (b) effective plastic strains on the $x$-$z$ plane.
Fig. 5.17. The effect of the thickness of the coating material on the normal pressure in the central plane $y = 0$.

5.3.2. Three inclusions in the coating material

In this section, the elastic-plastic behaviors of the film-substrate with three inhomogeneous inclusions in the coating are studied as shown in Fig. 5.18. The yield stress and Young’s modulus of the coating material are set to be $\sigma_{YC} = 600$ MPa and $E_C = 300$ GPa, respectively. Its thickness is set to be $d = 0.75a_0$. The three inhomogeneous inclusions ($\Omega_1$, $\Omega_2$ and $\Omega_3$) with the same side length $0.25a_0$ are centered at $(-0.5a_0, 0, 0.6a_0)$, $(0, 0, 0.6a_0)$ and $(0.5a_0, 0, 0.6a_0)$, respectively. Their yield stress is set to be $\sigma_{yi} = 900$ MPa. The effect of the Young’s modulus of the inhomogeneous inclusions on the surface pressure distribution and stress distribution is investigated.
Fig. 5.18. Schematic of a film-substrate with three inhomogeneous inclusions subjected to contact loading.

Fig. 5.19 shows the numerical results of various Young’s moduli of inhomogeneous inclusions, i.e., $E_i/E_s = 0.5, 1.0$ and $2.0$. It indicates that the presence of the inhomogeneous inclusions makes the surface pressure profiles more zigzag than the case of $E_i/E_s = 1.0$, in which no inclusion is considered. Moreover, this influence is more obvious when the inclusions are stiff. Figs. 5.20 and 5.21 demonstrate the von Mises stress and effective plastic strain distributions for the cases $E_i = 100$ GPa and $E_i = 400$ GPa, respectively. For the case $E_i = 100$ GPa, the maximum effective plastic strain occurs at both sides of the inclusion $\Omega_2$. While for the case $E_i = 400$ GPa, it occurs inside of the inclusions $\Omega_1$, $\Omega_2$ and $\Omega_3$. Moreover, the effective plastic strain increases from 0.4 to 0.65 with the decreasing of the Young’s moduli of inhomogeneous inclusions from 400 to 100 GPa.
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Fig. 5.19. The effect of the Young’s modulus of inhomogeneous inclusions on the normal pressure in the central plane $y = 0$.

Fig. 5.20. The effect of compliant inhomogeneous inclusions ($E_i = 100$ GPa) on the profiles of the (a) dimensionless von Mises stresses and (b) effective plastic strains on the $x$-$z$ plane.

Fig. 5.21. The effect of compliant inhomogeneous inclusions ($E_i = 400$ GPa) on the profiles of the (a) dimensionless von Mises stresses and (b) effective plastic strains on the $x$-$z$ plane.
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5.4. Summary

Coatings are commonly used to protect substrate materials in many engineering applications, such as gears, cams and cutting tools. As the protective layers, they are usually used as the surface reinforcements, which are beneficial to enhance the fatigue properties of materials and then improve their life duration. However, the substrate materials usually contain many types of microdefects, which may have the role to weaken the materials and eventually lead to fracture or structural damage [156-158].

In this chapter, the elastic-plastic behaviors of a film-substrate with inhomogeneous inclusions subjected to contact loading is studied by a semi-analytic solution. The coating material can be treated as an inhomogeneous inclusion with respect to the substrate. The increment of the effective plastic strains can be determined iteratively by a procedure involving a plasticity loop and an incremental loading process. The effect of the depths and Young’s moduli of the inhomogeneous inclusions, and the properties of the coating material on the surface pressure and substrate stress distributions, has been investigated.

The effect of the shape of the inclusions is demonstrated by the surface pressure distribution and the stress field. Moreover, in this study, the inhomogeneous inclusions with arbitrary shape can be investigated since they are modeled as many small cuboidal inhomogeneous inclusions. A good accuracy can be obtained as long as the discretization is fine enough.
Chapter 6 Elastic-plastic Model of a Half-space with Cracks and Inhomogeneous Inclusions

The elastic-plastic behaviors of materials are highly influenced by the presence of microdefects, especially when considering the effect of cracks. Due to the presence of cracks, the surface pressure and the substrate stress distribution of the material can be changed significantly. The contact loading condition will make this change more prominent. Therefore, in this chapter, the elastic-plastic behaviors of a half-space with cracks and inhomogeneous inclusions subjected to contact loading are investigated. The effective plastic strains can be determined by an iterative process based on the stress distribution and the von Mises yield criterion.

6.1. Methodology

6.1.1. Problem description and solution approach

In this chapter, we consider the contact system (two-dimensional problem \(xOz\)) of a cylinder \((E_R, \nu_R)\) and a half-space \((E_S, \nu_S)\) with inhomogeneous inclusions \((E_i, \nu_i)\) and cracks, as shown in Fig. 6.1(a). The external loading \(W\) is applied to the half-space surface by a cylinder with the radius \(R\). The half-space contains \(n\) arbitrarily-shaped inhomogeneous inclusions \(\Omega_\psi\) \((\psi = 1, 2, \cdots n)\), and \(m\) vertical or horizontal cracks \(\Gamma_\varphi\) \((\varphi = 1, 2, \cdots m)\). The elastic moduli of the inhomogeneous inclusions and the matrix material are denoted by \(C_{ijkl}^\psi\) and \(C_{ijkl}(i,j,k,l = 1,2,3)\), respectively.
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Fig. 6.1. Schematic of a half-space with cracks and inhomogeneous inclusions under contact loading.

The half-space contact problem with inhomogeneous inclusions and cracks can be transformed into a homogenous problem based on the EIM and DDT, as shown in Fig. 6.1(b). The computational domain D can be discretized into \( N_x \times N_z \) elements with the same size \( 2\Delta x \times 2\Delta z \), as shown in Fig. 6.2. Each element can be indexed by a sequence of two integers \([\alpha, \gamma]\) with \(0 \leq \alpha \leq N_x - 1\) and \(0 \leq \gamma \leq N_z - 1\).

Fig. 6.2. Discretization of the computational domain with \( \psi \) inhomogeneous inclusions and \( \varphi \) cracks into \( N_x \times N_z \) elements of the same size.
The current method assumes that the two surfaces of each subsurface crack are not in contact. In this way, the free-surface traction condition should be satisfied for each crack.

Based on the work done by Zhou and Wei [29] about the elastic behaviors of a half-space with inhomogeneous inclusions and cracks under contact loading, the governing equations for the inhomogeneous contact problem when considering the plastic behaviors of materials can be written as

\[(C_{ijkl}^{-1}C_{klimn} - 1)\sigma_{ij}^* + C_{ijkl}^\psi (\varepsilon_{kl}^* + \varepsilon_{kl}^{* *}) = (1 - C_{ijkl}^\psi C_{klimq}^{-1})(\sigma_{ij}^P + \sigma_{ij}^0 + \sigma_{ij}^c)\]  
(6.1a)

\[\psi = 1, 2, \cdots; i, j, k, l, m, q = 1, 2) \text{ within } \Omega_\psi,
\]

\[(\sigma_{ij}^P + \sigma_{ij}^* + \sigma_{ij}^c + \sigma_{ij}^0)n_j = 0 \]  
(6.1b)

\[\varphi = 1, 2, \cdots; i, j = 1, 2) \text{ along } \Gamma_\varphi,
\]

where \(\sigma_{ij}^P\) and \(\sigma_{ij}^*\) are the eigenstresses caused by the initial eigenstrain and equivalent eigenstrains in all the inclusions \(\Omega_\psi\); \(\sigma_{ij}^0\) is the stress applied by the external loading; \(\sigma_{ij}^c\) is the stress induced by all the cracks \(\Gamma_\varphi\); \(C_{ijkl}^\psi\) and \(C_{ijkl}\) are the elastic moduli of the inhomogeneous inclusion \(\Omega_\psi\) and the substrate, respectively; \(\varepsilon_{ij}^*\) is the equivalent eigenstrain; \(\varepsilon_{ij}^{* *}\) is the equivalent plastic strain; and \(n_j\) indicates the normal vector to crack surfaces.

In Eq. (6.1), the equivalent eigenstrain \(\varepsilon_{ij}^*\), the equivalent plastic strain \(\varepsilon_{ij}^{* *}\) and the stress induced by the cracks are unknowns. This stress can be calculated by integrating the dislocation densities, which are used to model the cracks along the crack lengths. In order to obtain these unknown strains and dislocation densities, the unknown contact area and surface pressure distribution need to be calculated firstly.
by a modified CGM. The detailed calculation method for the contact problem in a half-space with inhomogeneous inclusions and cracks under contact loading will be introduced in the following sections.

6.1.2. Contact problem for a half-space with inclusions and cracks

A two-dimensional half-space subjected to the cylindrical contact loading can be solved by a set of equations and inequalities, as described in Chapter 4. When the effect of the effective plastic strain, eigenstrains and cracks are taken into consideration, Eq. (4.5b) can be rewritten as:

$$h_\alpha = h_\alpha^i + \sum_{\xi=0}^{N_\xi-1} (Q_{\alpha-\xi}^n - \mu Q_{\alpha-\xi}^f) p_{\xi,0} + \sum_{\xi=0}^{N_\xi-1} \sum_{\zeta=0}^{N_\zeta-1} s_{a-\xi,y-\zeta} (\varepsilon^p_{\xi,\alpha} + \varepsilon^t_{\xi,\alpha} + \varepsilon^*_p)$$

$$+ \sum_{\xi=0}^{N_\xi-1} \sum_{\zeta=0}^{N_\zeta-1} \left( H_{a-\xi,y-\zeta}^{\perp} c_{\xi,\alpha}^\perp + K_{a-\xi,y-\zeta}^{\perp} d_{\xi,\alpha}^\perp + H_{a-\xi,y-\zeta}^{t} c_{\xi,\alpha}^t ight)$$

$$+ K_{a-\xi,y-\zeta}^{t} d_{\xi,\alpha}^t - \delta$$

where $p_{\alpha,0}$ represents the surface contact pressure on the element $[\alpha, 0]$; $h_\alpha$ denotes the gap between the two contact surfaces; $h_\alpha^i$ represents the initial gap; $Q_{\alpha-\xi}^n$ and $Q_{\alpha-\xi}^f$ are the coefficients relating the surface displacement to the normal pressure and tangential traction or friction, respectively; $s_{a-\xi,y-\zeta}$ are the coefficients relating the surface displacement to the initial eigenstrain $\varepsilon^p_{\xi,\alpha}$, the equivalent eigenstrain $\varepsilon^*_p$ and the effective equivalent plastic strain $\varepsilon^*_p$, and the detailed expressions of $Q_{\alpha-\xi}^n$, $Q_{\alpha-\xi}^f$ and $s_{a-\xi,y-\zeta}$ can be found in the work by Zhou et al. [14]; $c_{\xi,\alpha}^\perp$, $d_{\xi,\alpha}^\perp$, $c_{\xi,\alpha}^t$ and $d_{\xi,\alpha}^t$ denote the unknown dislocation densities; $H_{a-\xi,y-\zeta}^{\perp}$, $K_{a-\xi,y-\zeta}^{\perp}$, $H_{a-\xi,y-\zeta}^{t}$ and $K_{a-\xi,y-\zeta}^{t}$ are the coefficients relating the surface displacement to the dislocation densities, and their expressions can be found in the
work by Zhou and Wei [29]; \( \mu \) is the friction coefficient; and \( \delta \) is the relative rigid-body approach.

The contact area and surface pressure can be solved iteratively by a modified CGM. Due to the presence of the inhomogeneous inclusions and cracks, the surface displacement is significantly changed, which can in retune affect the contact area and surface pressure distribution. Therefore, with the initial inputs, an iterative process is used to calculate the surface pressure, the subsurface stress distribution and the surface displacement. This process will continue until the calculated surface displacement due to the inhomogeneous inclusions, cracks and accumulated plastic strains converges.

### 6.1.3. Numerical scheme

According to the governing equations for the elastic-plastic model of a half-space with inhomogeneous inclusions and cracks under contact loading, the effective plastic strain is added into the total strain when the stress of any point exceeds the yield strength of the corresponding material. According to the plastic flow rule, the plastic strain increment is determined by: 

\[
d \varepsilon_{ij}^p = d \lambda \frac{3 S_{ij}}{2 \sigma_{VM}},
\]

where \( d \lambda \) represents the plastic multiplier, \( S_{ij} \) is the deviatoric stress, and the von Mises equivalent stress \( \sigma_{VM} \) equals \( \sqrt{3 S_{ij} S_{ij} / 2} \).

After the surface contact pressure is obtained by solving a set of contact equations and inequations, the substrate stress field can be determined. The plastic domain is identified by the Newton-Raphson method and the \( J-2 \) criterion, and the equivalent eigenstrains and dislocation densities are then obtained. Afterwards, the surface displacement due to the inhomogeneous inclusions, cracks and accumulated plastic strains is calculated. As the surface displacement changes the surface contact
area and pressure distribution in return, the surface geometry is updated and the surface pressure is calculated again. A closed-loop is formed among the surface contact pressure, equivalent eigenstrains, accumulated plastic strains, dislocation densities and surface geometry. This loop will not be completed until the difference of the surface displacement between the two iterative steps is less than the prescribed error tolerance. Fig. 6.3 illustrates the flowchart of the elastic-plastic model of a half-space with cracks and inhomogeneous inclusions under contact loading.

![Flowchart](image)

**Fig. 6.3.** Flowchart for solving the elastic-plastic contact problem of a half-space with inhomogeneous inclusions and cracks.
6.2. Numerical results

6.2.1. Model verification

The linear hardening law is employed to analyze the elastic-plastic behavior of a material. The variable $E_t$ is the tangential modulus for the linear hardening law. When it equals zero, the material demonstrates elastic-perfectly plastic behavior. The radius of the rigid cylinder is set to be $R$, and an external loading $W$ is applied on it. The Hertz radius $a_0$ and peak pressure $p_0$ for the cylinder in two-dimensional contact with a homogeneous half-space depend on the external loading $W$ and the cylinder radius $R$. The material properties of the half-space are the Young’s modulus $E_s = 200$ GPa, the Poisson’s ratio $\nu = 0.3$ and the yield stress $\sigma_y = 600$ MPa. The computational domain is defined in the dimensions $-2a_0 \leq x \leq 2a_0$ and $0 \leq z \leq 2a_0$ with $80 \times 40$ unit grids.

The surface contact pressures based on the varied tangential modulus $E_t$ are plotted in Fig. 6.4(a). It can be found that the results from the current solution and the analytical Hertz solution match well. The FEM is a widely used numerical technique for solving engineering and mathematical problems. ABAQUS, ANSYS and NASTRAN are the commonly used commercial FEM tools. Many researchers have used this method to solve the elastoplastic behaviors of homogeneous or layered materials [43, 154] or the compression behavior of lattice structures [159]. Therefore, the present results of the case $E_t = 0.5E_s$ are compared with the FEM results reported by Dumas and Baronet [160]. They investigated the elastoplastic indentation behaviors of a half-space loaded by an infinitely long rigid circular cylinder with the assumption of plane strain deformation. The octahedral shear yield stress of the half-space is set to be $\tau_{yp}$ ($\tau_{yp} = \sigma_{yp}/\sqrt{3}$ with $\sigma_{yp}$ being the tensile yield stress). The parameter $b^*$ depends on the radius of the loading cylinder $R$ and
the material properties of the half-space \(b^* = 5.65\tau_{yp}/E\) with \(E\) being the Young’s modulus of the half-space). In the FEM simulation, the half-space is modeled by a rectangle with the dimensions much larger than the surface contact width. As shown in Fig. 6.4(b), a good agreement between the results of the present method and FEM can be found.
Before the study of the elastic-plastic behaviors of a half-space under contact loading, we need to determine the critical crack length $a_{cr}$ of a material. This critical length is a measure of the largest flaw which a material can tolerate before the unstable fracture occurs. According to the fracture toughness $K_{IC}$ and yield strength $\sigma_Y$ of the material, the range of the critical crack length can be determined by

$$a_{cr} \sim \left(\frac{K_{IC}}{\sigma_Y}\right)^2,$$

(6.3)

The fracture toughness $K_{IC}$ is a material constant and is independent of the size and geometry of the cracked body. Then, the critical crack length can be determined when the material is confirmed. In this study, all the crack lengths are set much smaller than the critical length. Therefore, all the cracks can be considered as stable, and there is no need to take the crack propagation into account.
In order to improve the computational efficiency, the FFT algorithm is utilized in the stage of numerical calculations. Therefore, the cracks beneath the contact surface are set to be horizontally or vertically oriented. A slant crack can be approximated by a collection of many small vertical and horizontal cracks.

6.2.2. One crack

Fig. 6.5 illustrates the schematic of a crack in a half-space subjected to contact loading. The material properties of the substrate and rigid cylinder are the same as those of the verified model. The tangential modulus $E_{ts}$ equals $0.5E_s$. These properties of the substrate and rigid cylinder for the numerical simulations are all the same in following sections. The crack $\Gamma_1$ has the length $a_0$ and is centered at $(0,a_0)$.

![Fig. 6.5. Schematic of a half-space with one crack subjected to contact loading.](image)

Fig. 6.6 illustrates the effect of the horizontal crack on the surface contact pressure distribution for various depths $h$. It shows that the presence of the crack significantly affects the surface contact pressure distribution. When the crack depth
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$h$ is less than $0.7a_0$, this effect becomes more and more significant and an obvious pressure drop at the center can be found in these cases. Moreover, it can also be found that the contact areas increase as the crack depth decreases. Fig. 6.7 plots the surface pressure distributions influenced by varied tangential modulus, i.e., $E_{ts} = E_s$, $E_{ts} = 0.75E_s$ and $E_{ts} = 0.5E_s$. The result of the case $E_t = E_s$, which represents the elastic material, shows a good agreement with that of the analytical Hertz solution. When the material is elastic-plastic, with the increment of the tangential modulus from $0.5E_s$ to $0.75E_s$, the surface contact pressure becomes more flat, and an obvious increment of the contact area can also be found.

![Graph showing surface pressure distributions with varying crack depths](image)

**Fig. 6.6.** The effect of the various crack depths $h$ on the surface pressure distribution.
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Fig. 6.7. The effect of the tangential modulus $E_{ts}$ on the surface pressure distribution.

Fig. 6.8 shows the effect of the crack length $l$ on the surface contact pressure distributions. It shows that the presence of the crack has significant influence on the surface contact pressure profiles. With the increment of the crack length from $0.5a_0$ to $1.5a_0$, it can be found that the surface contact pressure profiles become more flat and the peak value of the surface contact pressure decreases from $0.92p_0$ to $0.83p_0$. Moreover, an obvious increment tendency of the contact area can also be found.
Fig. 6.8. The effect of the various crack lengths $l$ on the surface contact pressure distribution.

6.2.3. Two horizontal cracks

In order to investigate the shielding or amplification effect of the distance between two cracks, a half-space with two cracks subjected to contact loading is considered as shown in Fig. 6.9. The two cracks $\Gamma_1$ and $\Gamma_2$ have the same length $a_0$, centered at $(0, 0.5a_0)$ and $(0, 1.5a_0)$, respectively.
Fig. 6.9. Schematic of two horizontal cracks in a half-space under contact loading.

Fig. 6.10 shows the effect of the distance between two cracks $d$ on the surface contact pressure distributions. The location of the crack $\Gamma_1$ is fixed and the distance $d$ varies by changing the depth of the crack $\Gamma_2$. It can be found that when the distance $d$ is small than $0.75a_0$, with the increment of the distance $d$ from $0.2a_0$ to $0.75a_0$, the contact pressure at the surface center increases dramatically from $0.208p_0$ to $0.252p_0$. Moreover, the peak pressure value appears at $x = \pm 0.7a_0$ and reduces from $0.934p_0$ to $0.92p_0$. However, when the distance $d$ exceeds $0.75a_0$, as the distance $d$ increases from $0.75a_0$ to $1.25a_0$, the contact pressure at the surface center decreases slightly from $0.252p_0$ to $0.247p_0$, and the peak pressure value also appears at $x = \pm 0.7a_0$ and increases from $0.92p_0$ to $0.949p_0$. Moreover, it can also be found that the contact area almost keeps unchanged with the increment of the distance $d$. 
Fig. 6.10. The effect of the distance between two cracks on the surface contact pressure distribution.

6.2.4. One horizontal crack and two inclusions

Fig. 6.11 shows the schematic of one horizontal crack and two inhomogeneous inclusions beneath a half-space subjected to contact loading. The crack $\Gamma_1$ has the length $0.5a_0$ and is centered at $(0, a_0)$. The two inhomogeneous inclusions $\Omega_1$ and $\Omega_2$ have the same side length $0.5a_0$, centered at $(-0.75a_0, a_0)$ and $(0.75a_0, a_0)$, respectively. Their yield stress is fixed at $\sigma_{yi} = 900$ MPa and the tangential modulus is set to be $0.5E_s$. The effect of the Young’s modulus of these inhomogeneous inclusions on the subsurface stress field and the effective plastic strain distribution is studied in this section.
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Fig. 6.11. Schematic of one horizontal crack and two inhomogeneous inclusions under contact loading.

The distributions of the effective plastic strain and the von Mises stress for the case $E_i = 0.5E_s$ are presented in Fig. 6.12. The results show that stress concentrations mainly occur around the crack tips, and the effective accumulative plastic strains occur at the corners of the inclusions and around the crack tips. Fig. 6.13 illustrates the distributions of the von Mises stresses and the effective plastic strain for the case $E_i = 2.0E_s$. It can be found that the maximum von Mises stresses occur not only around the crack tips but also at the edges of the inhomogeneous inclusions. The effective plastic strain inside the inclusions is smaller than that in the substrate. Moreover, as the Young’s modulus of inclusions increases from $0.5E_s$ to $2.0E_s$, the maximum effective plastic strain decreases from about 0.95 to 0.90.
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Fig. 6.12. Profiles of (a) the von Mises stresses and (b) the effective plastic strains for a horizontal crack and two compliant inhomogeneous inclusions ($E_i = 100$ GPa).

Fig. 6.13. Profiles of (a) the von Mises stresses and (b) the effective plastic strains for a horizontal crack and two stiffer inhomogeneous inclusions ($E_i = 400$ GPa)

6.2.5. One vertical crack and two inclusions

The schematic of two inhomogeneous inclusions and one vertical crack beneath a half-space subjected to contact loading is shown in Fig. 6.14. The crack $\Gamma_1$ has the length $a_0$ and is centered at $(0, a_0)$. The two inhomogeneous inclusions $\Omega_1$ and $\Omega_2$ have the same side length $a_0$, centered at $(-1.25a_0, a_0)$ and $(1.25a_0, a_0)$, respectively. Their material properties are the same as those in section 6.2.4.
Fig. 6.14. Schematic of one vertical crack and two inhomogeneous inclusions under contact loading.

The effect of the stiff inclusions and the compliant inclusions on the von Mises stresses and the effective plastic strains is presented in Figs. 6.15 and 6.16, respectively. For the compliant inclusions $E_i = 0.5E_s$, the stress concentrations can be found at the substrate around the upper crack tip and outside the corners of the inclusions (near the upper crack tip). For the stiff inclusions $E_i = 2.0E_s$, the stress concentrations mainly appear along the sides of the inclusions. Moreover, it can also be found that the effective plastic strains in the compliant case are more obvious in the substrate than those in the stiff case. As the Young’s modulus of the inhomogeneous inclusions increases from $0.5E_s$ to $2.0E_s$, the maximum effective plastic decreases from about 1.0 to 0.9.
6.3. **Summary**

In this chapter, the elastic-plastic behaviors of a half-space with cracks and inhomogeneous inclusions under contact loading are studied. When the subsurface stresses exceed the yield strength of the corresponding material, the plastic strains should be obtained iteratively by a plasticity loop when the surface displacement induced by the subsurface defects and contact loading converges. Based on the von Mises yield criterion and substrate stress fields, the plastic zone shape of crack tips is calculated, which is significantly influenced by the Young’s modulus of inclusions, the crack depth, the crack length and the material properties of the substrate. In order to make the investigations close to the real cases, the elastic-plastic behaviors of materials with horizontal or vertical cracks are studied.

In this study, the effective plastic strain is added to the total strain and then

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**Fig. 6.15.** Profiles of (a) the von Mises stresses and (b) the effective plastic strains for a vertical crack and two compliant inhomogeneous inclusions ($E_i = 100$ GPa).

**Fig. 6.16.** Profiles of (a) the von Mises stresses and (b) the effective plastic strains for a vertical crack and two stiff inhomogeneous inclusions ($E_i = 400$ GPa).

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influences the substrate stress fields. According to the contours of the effective plastic strain, it can be found that the plastic zones can significantly affect the stress distribution of the matrix material.

Due to the assumptions of the cracks and the contact model, the solution for the cracks touching the contact surface is beyond the scope of the current developed model. Moreover, when the distance between two cracks becomes much smaller before they are overlapped, the present model cannot provide a prediction since cracks are modeled based on the setting of the discretization domain. When the distance between two cracks is too small to be overlapped, they would be treated as a single crack to obtain the simulation results in the current model.
Chapter 7 Conclusions and Recommendations

In this chapter, the main conclusions based on the works conducted during this PhD study are drawn and the future works are recommended.

7.1. Conclusions

The micromechanics investigation of solid materials with defects is a complex problem due to the presence of the defects, especially for the elastic-plastic behaviors of materials. When taking the contact problem into account, this investigation becomes more complicated since the stress concentrations and the material yielding near the contact area are easily caused. Generally, it is extremely difficult to derive an analytic solution to study the elastic-plastic behaviors of materials when considering the defects and contact loading, and thus a semi-analytic solution is developed.

By means of the Dugdale crack model and the elastic-plastic contact model, the major contribution of this thesis is that several semi-analytic solutions are proposed to investigate the elastic-plastic behaviors of materials with defects under different loading conditions. It is of great importance to investigate the mechanical behaviors of materials with defects for the minimization of potential damage and failure of the components. The detailed conclusions can be summarized as follows.

In this thesis, the plastic zone sizes of crack tips in an infinite space under the remote tensile loading are first investigated. Due to considering the influence of inhomogeneous inclusions or loading conditions, the modified Dugdale model is used to calculate the plastic zone sizes of crack tips. It is found that the Young’s moduli and positions of the inhomogeneous inclusions have significant influences
on the plastic zone sizes of crack tips. Moreover, it is also found that the climb dislocation densities along the crack length are anti-symmetric about the crack center and the density value at the effective crack tips decreases with the increase of the Young’s modulus of the inhomogeneous inclusions. The normal CTOD can be calculated by summing the climb dislocation densities along the effective crack length and its distribution is symmetric about the crack center.

Afterwards, the plastic zone sizes of crack tips in a half-space under contact loading are studied. This inhomogeneous contact problem is solved iteratively using a conjugate gradient method until the surface displacement due to the contact load and the cracks converges. It is found that the plastic zone size of crack tips decreases with the increase of the material yield strength and the crack depth. While it increases with the increase of the original crack length and the external loading.

Then, the elastic-plastic behaviors of a film-substrate with inhomogeneous inclusions under contact loading are investigated. The coating material can be regarded as a homogeneous inclusion with respect to the substrate based on the EIM. The effective plastic strain evolution can be determined by a plasticity loop and the plastic flow rule. The elastic-plastic model for the film-substrate is validated by the analytical results of O’Sullivan and King [155]. It can be found that the effect of the inclusion on the surface pressure and subsurface stress distributions is more obvious when the inclusion is close to the interface between the coating and the substrate. Moreover, the stress concentrations can be found around the inhomogeneous inclusions, especially when the inclusions are located at the coating material.

Finally, the elastic-plastic behaviors of a half-space with cracks and inhomogeneous inclusions subjected to contact loading are also studied. Both horizontal and vertical cracks relative to the loading direction are considered. A
group of numerical examples are conducted to investigate the effect of the material properties of inclusions and cracks on the subsurface von Mises stress and contact pressure distributions. It can be found that the crack depth $h$ can significantly change the surface contact pressure distribution and this effect becomes more obvious when cracks are close enough to the contact surface.

In the current study, some theoretical expressions of the proposed models need to be given as follows. Firstly, the plastic strips are investigated under the remote tensile stress, the prescribed pressure and contact loading, based on the modified Dugdal model. Generally, the mixed-mode loadings will cause the plastic strips to deviate from the crack plane since the maximum von Mises stress may occur at an angle from the crack plane. However, it should be noted that the resultant stress at an angle from the crack plane cannot exceed the yield strength of the matrix material. Therefore, in this study, the external loading conditions will not cause the plastic strips to deviate from the crack plane obviously.

Secondly, when considering the plastic zone size of cracks, the distribution of defects is special due to the Dugdale crack model. However, when considering the elastic-plastic behaviors of materials with inhomogeneous inclusions and cracks, the investigation is to determine the elastic-plastic properties of the materials based on the von Mises yield criterion. Therefore, for the elastic-plastic models, the distributions of the inhomogeneous inclusions and cracks are arbitrary.

Moreover, the semi-analytic solution directly handles the square inhomogeneous inclusions and also solves the unknown equivalent eigenstrains with the square inclusions. Whether these square inclusions are decomposed from a single or multiple spaced inhomogeneous inclusions does not create any difference to the solution. However, the final solution of the equivalent eigenstrains reflects
their difference. Therefore, in this study, only square inclusions are investigated.

Finally, for the elastic-plastic models of a half-space or a film-substrate with defects under contact loading, the effective plastic strain increment is calculated when the surface displacement due to the coating material, embedded defects and contact loading converges. Therefore, the present models cannot be used to calculate the effective elastic-plastic properties.

Though there are some limitations of this study, the proposed semi-analytic solutions can still provide important insights in the mechanics analysis of materials with defects. One strength of these semi-analytic solutions is that the computational domain in the FEM is much larger than that in the present method when consideration the effect of the defects, coating material and contact loading. Therefore, the iterative process to obtain the unknown eigenstrain, effective plastic strain, surface area and pressure distribution would save much time in this study. Moreover, the present solution is verified with not only the corresponding FEM results but also the analytical results. A good agreement can be found among them.

The other strength of these semi-analytic solutions is that they can deal with the situation of multiple cracks and inhomogeneous inclusions in the same way as treating a single crack or a single inclusion without adding computational difficulties. This is because the inhomogeneous inclusions and cracks have been decomposed into many square inhomogeneous inclusions and crack segments in a discretized domain at the beginning of the simulation. Moreover, their tips easily yield when the materials are subjected to the external loading since the stresses at crack tips are large even though the applied loading is very small. Therefore, a more accurate description of materials with cracks could be obtained when considering their plastic zones, which is beneficial to analyze the crack initiation and
propagation.

In summary, the semi-analytic solutions developed in this thesis are used to obtain an accurate analysis for the solid materials with defects and provide a reasonable fundamental for potential applications of the mechanical components.

7.2. Recommendations

The above semi-analytic solutions are developed for the elastic-plastic behaviors of materials with multiple inhomogeneous inclusions and cracks under different loading conditions. However, in the real cases, the mechanical properties of materials with defects can be influenced by many factors, such as the lubrication conditions, the loading types, the surface roughness, investigation models for the crack-tip plasticity, or the crack propagation. Therefore, the following works are recommended here to further investigate the mechanical properties of materials with defects.

Firstly, the contact surfaces are commonly flawed by roughness. The presence of the surface roughness may induce very high local pressure and significantly influence the surface pressure distribution. For a better understanding of the contact behaviors with rough surfaces, a further study should be extended to investigate the effect of the surface roughness on the elastic-plastic behaviors of materials with defects under contact loading.

Secondly, friction phenomenon is unavoidable in the engineering components. In order to alleviate the material damage, lubrications are widely used between the loading body and the substrate material to prevent the surfaces from direct contact. According to the previous studies on the lubrication problems, the elastic-plastic behaviors of materials with defects under the complex lubrication conditions can be
solved based on the Reynolds equations and Barus law.

Finally, the mechanical components are usually applied under cyclic loading in the real cases. This loading condition can induce crack initiation, crack propagation and finally cause the material failure. According to the Paris law and the maximum hoop stress criterion, the previous works just focused on the fatigue crack growth directions. However, the elastic-plastic behaviors of materials are not taken into consideration. The further study can be conducted on the elastic-plastic behaviors of materials with defects under cyclic loading.
Appendix A

In the inhomogeneous infinite space problem, the total strain $\varepsilon_{ij}$ at any point within the inhomogeneous inclusion $\Omega_\varphi$ contains two parts: the elastic strain $\varepsilon_{ij}^e$ and the initial eigenstrain $\varepsilon_{ij}^P$. The detailed expression can be given by $\varepsilon_{ij} = \varepsilon_{ij}^e + \varepsilon_{ij}^P$. According to Hooke’s law, the stress can be expressed as $\sigma_{ij} = C_{ijkl}^\psi (\varepsilon_{kl} - \varepsilon_{kl}^P)$. In each equivalent homogeneous inclusion $\Omega_\varphi$, $\varepsilon_{ij} = \varepsilon_{ij}^e + \varepsilon_{ij}^P + \varepsilon_{ij}^*$, where $\varepsilon_{ij}^*$ is the equivalent eigenstrain. Therefore, according to Hooke’s law, the stress can be expressed as $\sigma_{ij} = C_{ijkl}^\psi (\varepsilon_{kl} - \varepsilon_{kl}^* - \varepsilon_{kl}^P)$. The combination of these two stress-strain formulae gives the stress $\sigma_{ij}$ at any point in $\Omega_\varphi$ as $\sigma_{ij} = C_{ijkl}^\psi (C_{klm}^\psi - 1^\psi)$. On the other hand, the stress $\sigma_{ij}$ at any point in each equivalent inclusion $\Omega_\varphi$ is given by $\sigma_{ij} = \sigma_{ij}^* + \sigma_{ij}^P + \sigma_{ij}^c + \sigma_{ij}^0$, where $\sigma_{ij}^p$ and $\sigma_{ij}^*$ are the eigenstresses induced by all the initial eigenstrains $\varepsilon_{ij}^p$ and all the equivalent eigenstrains $\varepsilon_{ij}^*$, respectively; $\sigma_{ij}^c$ and $\sigma_{ij}^0$ are the stresses caused by all the cracks and remote loading, respectively. The combination of the two stress expressions leads to the following governing equations:

\[
C_{ijkl}^\psi C_{klm} (\sigma_{ij}^p + \sigma_{ij}^* + \sigma_{ij}^c + \sigma_{ij}^0 - \sigma_{ij} - \sigma_{ij}^* - \sigma_{ij}^c - \sigma_{ij}^0 + C_{ijkl}^\psi \varepsilon_{ij}^* = 0
\]

\[
(\psi = 1, 2, \ldots, w; i, j, k, l, m, q = 1, 2) \text{ within } \Omega_\varphi,
\]

For the crack model, the two surfaces of a crack are assumed not to be in contact with each other. Thus, the conditions of free surface tractions along the normal and tangential directions should be satisfied for each crack. Therefore, the governing equations can be established:
\[ \sigma_{ij}^P + \sigma_{ij}^* + \sigma_{ij}^C + \sigma_{ij}^0 = 0 \quad (i, j = 1, 2) \text{ along } \Gamma_\varphi, \] (A2)

where \( i = 1 \) for a crack perpendicular to the \( x \)-axis and \( i = 2 \) for a crack perpendicular to the \( y \)-axis.

The calculation method for the eigenstress field is obtained based on a closed-form solution proposed by Chiu [97]. In this solution, the elastic strain is determined according to the geometric equation on a continuous displacement field. Then, the strain compatibility equations are satisfied. The detailed method to calculate the strain and stress is introduced as follow.

A Cartesian coordinate system \((x_1, x_2, x_3)\) is attached to the space and its origin is set at the center of the cuboid, which has side lengths \(2\Delta_1\), \(2\Delta_2\) and \(2\Delta_3\) along the axes \(x_1\), \(x_2\) and \(x_3\), respectively. Given an observation point at \(Q(\xi_1, \xi_2, \xi_3)\), we define the vectors which link the corners of the cuboid to this point as follows:

\[ C_m = (y_1^m, y_2^m, y_3^m), \] (A3)

where

\begin{align*}
C_1 &= (\xi_1 - \Delta_1, \xi_2 - \Delta_2, \xi_3 - \Delta_3), \quad \text{(A4a)} \\
C_2 &= (\xi_1 + \Delta_1, \xi_2 - \Delta_2, \xi_3 - \Delta_3), \quad \text{(A4b)} \\
C_3 &= (\xi_1 + \Delta_1, \xi_2 + \Delta_2, \xi_3 - \Delta_3), \quad \text{(A4c)} \\
C_4 &= (\xi_1 - \Delta_1, \xi_2 + \Delta_2, \xi_3 - \Delta_3), \quad \text{(A4d)} \\
C_5 &= (\xi_1 - \Delta_1, \xi_2 + \Delta_2, \xi_3 + \Delta_3), \quad \text{(A4e)} \\
C_6 &= (\xi_1 - \Delta_1, \xi_2 - \Delta_2, \xi_3 + \Delta_3), \quad \text{(A4f)} \\
C_7 &= (\xi_1 + \Delta_1, \xi_2 - \Delta_2, \xi_3 + \Delta_3), \quad \text{(A4g)} \\
C_8 &= (\xi_1 + \Delta_1, \xi_2 + \Delta_2, \xi_3 + \Delta_3). \quad \text{(A4h)}
\end{align*}
If the cuboidal inclusion contains constant unit normal eigenstrain $\varepsilon_{11}^P$, i.e. $\varepsilon_{11}^P = 1$ and other components are zero, the elastic strain at $Q(\xi_1, \xi_2, \xi_3)$ due to the inclusion is given by

$$\varepsilon_{1111} = \frac{1}{8\pi^3} \sum_{m=1}^{8} \left[ D_{1111}^m - \frac{2 - \nu}{1 - \nu} \left( D_{1111}^m + D_{1113}^m \right) \right] - H(Q), \quad (A5a)$$

$$\varepsilon_{2211} = -\frac{1}{8\pi^3} \sum_{m=1}^{8} \left[ -D_{1122}^m + \frac{\nu}{1 - \nu} \left( D_{2222}^m + D_{2233}^m \right) \right] \quad (A5b)$$

$$\varepsilon_{3311} = -\frac{1}{8\pi^3} \sum_{m=1}^{8} \left[ -D_{1133}^m + \frac{\nu}{1 - \nu} \left( D_{3333}^m + D_{3333}^m \right) \right] \quad (A5c)$$

$$\varepsilon_{1211} = \frac{1}{8\pi^3} \sum_{m=1}^{8} \left[ \frac{\nu}{1 - \nu} D_{1112}^m + \frac{1 + \nu}{1 - \nu} \left( D_{2221}^m + D_{3312}^m \right) \right] \quad (A5d)$$

$$\varepsilon_{1311} = \frac{1}{8\pi^3} \sum_{m=1}^{8} \left[ \frac{\nu}{1 - \nu} D_{1113}^m + \frac{1 + \nu}{1 - \nu} \left( D_{3331}^m + D_{3312}^m \right) \right] \quad (A5e)$$

$$\varepsilon_{2311} = \frac{1}{8\pi^3} \sum_{m=1}^{8} \frac{\nu}{1 - \nu} \left( D_{2233}^m + D_{3332}^m \right) \quad (A5f)$$

If the cuboidal inclusion contains constant unit shear eigenstrain $\varepsilon_{12}^P$, i.e. $\varepsilon_{12}^P = \varepsilon_{21}^P = 1$ and the other components are zero, the elastic strain at $Q(\xi_1, \xi_2, \xi_3)$ is given by

$$\varepsilon_{1112} = \frac{1}{8\pi^3} \sum_{m=1}^{8} \left[ -\frac{2\nu}{1 - \nu} D_{1112}^m + 2 \left( D_{2221}^m + D_{3312}^m \right) \right] \quad (A6a)$$

$$\varepsilon_{2212} = \frac{1}{8\pi^3} \sum_{m=1}^{8} \left[ -\frac{2\nu}{1 - \nu} D_{1122}^m + 2 \left( D_{1112}^m + D_{3312}^m \right) \right] \quad (A6b)$$

$$\varepsilon_{3312} = \frac{1}{8\pi^3} \sum_{m=1}^{8} \frac{-2\nu}{1 - \nu} D_{3312}^m \quad (A6c)$$
\[
\varepsilon_{1212} = \frac{1}{8\pi^3} \sum_{m=1}^{8} \left[ \frac{-2\nu}{1-\nu} D_{1122}^m + D_{1111}^m + D_{2222}^m + D_{1133}^m + D_{2233}^m \right] - H(Q),
\]
(A6d)

\[
\varepsilon_{1312} = \frac{1}{8\pi^3} \sum_{m=1}^{8} \frac{-1 + \nu}{1-\nu} D_{1123}^m + D_{2223}^m + D_{3332}^m.
\]
(A6e)

\[
\varepsilon_{2312} = \frac{1}{8\pi^3} \sum_{m=1}^{8} \frac{-1 + \nu}{1-\nu} D_{2213}^m + D_{1113}^m + D_{3331}^m.
\]
(A6f)

In these equations, \( H(Q) = 1 \) if the point \( Q \) is inside the cuboid and \( H(Q) = 0 \) otherwise. Four of the functions \( D_{ijkl}^m \) are defined as follows:

\[
D_{1111}^m = 2\pi^2 \left[ \tan^{-1} \left( \frac{y_2^m y_3^m}{y_1^m R_m} \right) \right] - \frac{y_1^m y_2^m y_3^m}{2R} \left( \frac{1}{(y_1^m)^2 + (y_2^m)^2} + \frac{1}{(y_1^m)^2 + (y_3^m)^2} \right),
\]
(A7a)

\[
D_{1112}^m = -\pi^2 \left[ \text{sign}(y_3^m) \right] \times \ln \left( \frac{R_m + |y_3^m|}{((y_1^m)^2 + (y_2^m)^2)^{1/2} + (y_3^m)^2 + (y_3^m)^2 R_m} \right),
\]
(A7b)

\[
D_{1122}^m = \frac{\pi^2 y_1^m y_2^m y_3^m}{((y_1^m)^2 + (y_2^m)^2) R_m},
\]
(A7c)

\[
D_{1123}^m = -\frac{\pi^2 y_1^m}{R_m},
\]
(A7d)

where

\[
R_m = \sqrt{(y_1^m)^2 + (y_2^m)^2 + (y_3^m)^2}.
\]
(A8)

The rest of the functions \( D_{ijkl}^m \) are obtained by circular permutation of the subscripts in above equations.
The elastic strain at $Q(\xi_1, \xi_2, \xi_3)$ due to the cuboidal inclusions which contains other unit normal or shear eigenstrains can also be obtained by circular permutation of the subscripts.

Finally, according to Hooke’s law, the stress at $Q(\xi_1, \xi_2, \xi_3)$ due to the cuboidal inclusion can be obtained from the elastic strain. Therefore, the functions $B_{ijkl}$ relating the stress to the constant eigenstrain in a cuboidal inclusion centered at the origin in an infinite space are determined.

According to the discretization method in the computational domain, the governing equations (A1) and (A2) can be given by

\[
\begin{align*}
(C_{\alpha,\beta}C^{-1} - 1) & \left[ \sum_{\zeta=0}^{N_x-1} \sum_{\xi=0}^{N_y-1} \left( B_{a-\xi,\beta-\zeta} \varepsilon_{\xi,\zeta}^P + B_{a-\xi,\beta-\zeta} \varepsilon_{\xi,\zeta}^P \right) 
+ \frac{2\mu}{\pi(\kappa + 1)} \sum_{\zeta=0}^{N_x-1} \sum_{\xi=0}^{N_y-1} \left( E_{a-\xi,\beta-\zeta}^P + E_{a-\xi,\beta-\zeta}^P + F_{a-\xi,\beta-\zeta}^P + F_{a-\xi,\beta-\zeta}^P \right) \right] 
+ C_{\alpha,\beta} \varepsilon_{\alpha,\beta} \\
&= 0
\end{align*}
\]

\[
\begin{align*}
\sum_{\zeta=0}^{N_x-1} \sum_{\xi=0}^{N_y-1} \left( B_{a-\xi,\beta-\zeta} \varepsilon_{\xi,\zeta}^P + B_{a-\xi,\beta-\zeta} \varepsilon_{\xi,\zeta}^P \right) 
+ \frac{2\mu}{\pi(\kappa + 1)} \sum_{\zeta=0}^{N_x-1} \sum_{\xi=0}^{N_y-1} \left( E_{a-\xi,\beta-\zeta}^P + E_{a-\xi,\beta-\zeta}^P + F_{a-\xi,\beta-\zeta}^P + F_{a-\xi,\beta-\zeta}^P \right) = 0
\end{align*}
\]

where the coefficients $B_{a-\xi,\beta-\zeta}$, which relates the eigenstresses $\sigma_{\alpha,\beta}^P$ and $\sigma_{\alpha,\beta}^*$
at the observation point \((x_\alpha, y_\beta)\) in the square element \([\alpha, \beta]\) to the initial
eigenstrains \(\varepsilon^{p}_{\xi, \zeta}\) and equivalent eigenstrains \(\varepsilon^{*}_{\xi, \zeta}\) in the element \([\xi, \zeta]\),
respectively; \(E_{a-\xi, \beta-\zeta}^{+}, F_{a-\xi, \beta-\zeta}^{+}, E_{a-\xi, \beta-\zeta}^{-}\) and \(F_{a-\xi, \beta-\zeta}^{-}\) are the influence
coefficients relating the stresses to the dislocation density parameters \(c^{+}_{\xi, \zeta}, d^{+}_{\xi, \zeta},
c^{-}_{\xi, \zeta}\) and \(d^{-}_{\xi, \zeta}\), respectively, which can be expressed as follows according to the
work [161].

\[
E_{11}^{+}(x, y) = \frac{2 \mu}{\pi (\kappa + 1)} \left\{ \frac{\Delta_x y^2}{(x - \Delta_x)^2 + y^2} + \frac{\Delta_x y^2}{(x + \Delta_x)^2 + y^2} \right. \\
+ \frac{x}{2} \ln \left[ \frac{(x - \Delta_x)^2 + y^2}{(x + \Delta_x)^2 + y^2} \right] \\
\left. + 2y \left[ \tan^{-1} \left( \frac{x - \Delta_x}{y} \right) - \tan^{-1} \left( \frac{x + \Delta_x}{y} \right) \right] + 2 \Delta_x \right\}, \tag{A10a}
\]

\[
F_{11}^{+}(x, y) = \frac{2 \mu}{\pi (\kappa + 1)} \left\{ \frac{y^2}{(x + \Delta_x)^2 + y^2} - \frac{y^2}{(x - \Delta_x)^2 + y^2} \right. \\
- \frac{1}{2} \ln \left[ \frac{(x - \Delta_x)^2 + y^2}{(x + \Delta_x)^2 + y^2} \right] \right. \\
\left. - 1 \right\}, \tag{A10b}
\]

\[
E_{22}^{+}(x, y) = \frac{2 \mu}{\pi (\kappa + 1)} \left\{ \frac{\Delta_x (x + \Delta_x)^2}{(x + \Delta_x)^2 + y^2} + \frac{\Delta_x (x - \Delta_x)^2}{(x - \Delta_x)^2 + y^2} \right. \\
+ \frac{x}{2} \ln \left[ \frac{(x - \Delta_x)^2 + y^2}{(x + \Delta_x)^2 + y^2} \right] \right. \\
\left. + \frac{x}{2} \ln \left[ \frac{(x - \Delta_x)^2 + y^2}{(x + \Delta_x)^2 + y^2} \right] \right\}, \tag{A10c}
\]

\[
F_{22}^{+}(x, y) = \frac{2 \mu}{\pi (\kappa + 1)} \left\{ \frac{y^2}{(x - \Delta_x)^2 + y^2} - \frac{y^2}{(x + \Delta_x)^2 + y^2} \right. \\
- \frac{1}{2} \ln \left[ \frac{(x - \Delta_x)^2 + y^2}{(x + \Delta_x)^2 + y^2} \right] \right. \\
\left. - \frac{1}{2} \ln \left[ \frac{(x - \Delta_x)^2 + y^2}{(x + \Delta_x)^2 + y^2} \right] \right\}. \tag{A10d}
\]
\[
E_{12}^*(x, y) = \frac{2\mu y}{\pi(\kappa + 1)} \left\{ \frac{(x^2 - \Delta_x x + y^2)}{(x - \Delta_x)^2 + y^2} - \frac{(x^2 + \Delta_x x + y^2)}{(x + \Delta_x)^2 + y^2} \right\} \\
+ \frac{1}{2} \ln \left[ \frac{(x - \Delta_x)^2 + y^2}{(x + \Delta_x)^2 + y^2} \right].
\]

\[(A10e)\]

\[
F_{12}^*(x, y) = \frac{2\mu}{\pi(\kappa + 1)} \left\{ \frac{y(x - \Delta_x)}{(x - \Delta_x)^2 + y^2} - \frac{y(x + \Delta_x)}{(x + \Delta_x)^2 + y^2} \right\}.
\]

\[(A10f)\]

\[
E_{11}^*(x, y) = \frac{2\mu}{\pi(\kappa + 1)} \left\{ y \left[ \frac{(y^2 + \Delta_x x + x^2)}{(x + \Delta_x)^2 + y^2} - \frac{(y^2 - \Delta_x x + x^2)}{(x - \Delta_x)^2 + y^2} \right] \right\} \\
- \frac{3y}{2} \ln \left[ \frac{(x - \Delta_x)^2 + y^2}{(x + \Delta_x)^2 + y^2} \right].
\]

\[(A11a)\]

\[
F_{11}^*(x, y) = \frac{2\mu}{\pi(\kappa + 1)} \left\{ \frac{y(x + \Delta_x)}{(x + \Delta_x)^2 + y^2} - \frac{y(x - \Delta_x)}{(x - \Delta_x)^2 + y^2} \right\} \\
+ 2\tan^{-1}\left( \frac{x - \Delta_x}{y} \right) - 2\tan^{-1}\left( \frac{x + \Delta_x}{y} \right).
\]

\[(A11b)\]

\[
E_{22}^*(x, y) = \frac{2\mu y}{\pi(\kappa + 1)} \left\{ \frac{(y^2 - \Delta_x x + x^2)}{(x - \Delta_x)^2 + y^2} - \frac{(y^2 + \Delta_x x + x^2)}{(x + \Delta_x)^2 + y^2} \right\} \\
+ \frac{1}{2} \ln \left[ \frac{(x - \Delta_x)^2 + y^2}{(x + \Delta_x)^2 + y^2} \right].
\]

\[(A11c)\]

\[
F_{22}^*(x, y) = \frac{2\mu}{\pi(\kappa + 1)} \left\{ \frac{y(x - \Delta_x)}{(x - \Delta_x)^2 + y^2} - \frac{y(x + \Delta_x)}{(x + \Delta_x)^2 + y^2} \right\}.
\]

\[(A11d)\]

\[
E_{12}^*(x, y) = -\frac{2\mu}{\pi(\kappa + 1)} \left\{ \frac{\Delta_x y^2}{(x - \Delta_x)^2 + y^2} + \frac{\Delta_x y^2}{(x + \Delta_x)^2 + y^2} \right\} \\
+ \frac{x}{2} \ln \left[ \frac{(x - \Delta_x)^2 + y^2}{(x + \Delta_x)^2 + y^2} \right].
\]

\[(A11e)\]
\[
F_{12}^\perp(x, y) = \frac{2\mu}{\pi(\kappa + 1)} \left\{ \frac{y^2}{(x + \Delta_x)^2 + y^2} - \frac{y^2}{(x - \Delta_x)^2 + y^2} \right\} \\
- \frac{1}{2} \ln \left[ \frac{(x - \Delta_x)^2 + y^2}{(x + \Delta_x)^2 + y^2} \right].
\] (A11f)

The unknown equivalent eigenstrains and dislocation densities can be obtained by solving the governing equation using the CGM. The FFT algorithm is applied to improve the computational efficiency.
The influence coefficients for horizontal cracks relating the stresses to the climb and glide dislocations are given as

\[ F_{11}^1 = -\frac{1}{2} \ln \left[ \frac{(a-x)^2 + (z+\eta)^2}{(a-x)^2 + (z-\eta)^2} \right] + 1 \ln \left[ \frac{(a+x)^2 + (z+\eta)^2}{(a+x)^2 + (z-\eta)^2} \right] \]

\[ + \frac{(\eta - z)^2}{(x-a)^2 + (\eta - z)^2} - \frac{(\eta - z)^2}{(x+a)^2 + (\eta - z)^2} \]

\[ + \frac{3\eta^2 + 4\eta z - z^2}{(x-a)^2 + (\eta + z)^2} - \frac{3\eta^2 + 4\eta x - z^2}{(x+a)^2 + (\eta + z)^2} \]

\[ - \frac{4\eta z(\eta + \eta)^2}{[(x-a)^2 + (\eta + z)^2]^2} + \frac{4\eta z(\eta + \eta)^2}{[(x+a)^2 + (\eta + z)^2]^2} \]

\[ E_{11}^1 = -\frac{x}{2} \left\{ \ln \left[ \frac{(a-x)^2 + (z+\eta)^2}{(a-x)^2 + (z-\eta)^2} \right] - \ln \left[ \frac{(a+x)^2 + (z+\eta)^2}{(a+x)^2 + (z-\eta)^2} \right] \right\} \]

\[ - \frac{2\eta [((a+x)(\eta + z)^2 - (a-x)^3]}{(a-x)^2 + (\eta + z)^2} + \frac{a(\eta - z)^2}{(a+x)^2 + (\eta - z)^2} \]

\[ - \frac{2\eta [((a-x)(\eta + z)^2 - (a+x)^3]}{(a+x)^2 + (\eta + z)^2} + \frac{a(\eta - z)^2}{(a-x)^2 + (\eta - z)^2} \]

\[ - 2(\eta - z) \left[ \tan^{-1} \left( \frac{a-x}{\eta - z} \right) + \tan^{-1} \left( \frac{a-x}{\eta + z} \right) + \tan^{-1} \left( \frac{a+x}{\eta - z} \right) + \tan^{-1} \left( \frac{a+x}{\eta + z} \right) \right] \]

\[ + \frac{a(z^2 - 4\eta z - 3\eta^2)}{(a-x)^2 + (\eta + z)^2} \]

\[ - \frac{a(z^2 - 4\eta z - 3\eta^2)}{(a+x)^2 + (\eta + z)^2} \]
\[
F_{22}^\perp = \frac{z^2 + \eta^2}{(x - a)^2 + (\eta + z)^2} - \frac{z^2 + \eta^2}{(x + a)^2 + (\eta + z)^2} \\
- \frac{(\eta - z)^2}{(x - a)^2 + (\eta - z)^2} \\
+ \frac{1}{2} \ln \left[ \frac{(a - x)^2 + (z - \eta)^2}{(a - x)^2 + (z + \eta)^2} \right] - \frac{1}{2} \ln \left[ \frac{(a + x)^2 + (z - \eta)^2}{(a + x)^2 + (z + \eta)^2} \right] + (B3)
\]

\[
E_{22}^\perp = \frac{2\eta z[(a + x)(z + \eta)^2 - (a - x)^3]}{[(a - x)^2 + (\eta + z)^2]^2} \\
+ \frac{2\eta z[(a - x)(z + \eta)^2 - (a + x)^3]}{[(a + x)^2 + (\eta + z)^2]^2} \\
+ \frac{x}{2} \left\{ \ln \left[ \frac{(a - x)^2 + (z - \eta)^2}{(a - x)^2 + (z + \eta)^2} \right] - \ln \left[ \frac{(a + x)^2 + (z - \eta)^2}{(a + x)^2 + (z + \eta)^2} \right] \right\} + (B4)
\]

\[
F_{12}^\perp = -\frac{8\eta^2 z(a - x)[(a - x)^2 + \eta^2 - z^2]}{[(a - x)^2 + (\eta - z)^2][(a - x)^2 + (\eta + z)^2]} \\
- \frac{8\eta^2 z(a + x)[(a + x)^2 + \eta^2 - z^2]}{[(a + x)^2 + (\eta - z)^2][(a + x)^2 + (\eta + z)^2]} + (B5)
\]
\[ E_{12}^4 = \frac{5\eta z^2 + 7\eta^2 z + \eta x^2 + ax(\eta - z) - zx^2 + \eta^3 - z^3}{(a + x)^2 + (\eta + z)^2} \]
\[ - \frac{5\eta z^2 + 7\eta^2 z + \eta x^2 - ax(\eta - z) - zx^2 + \eta^3 - z^3}{(a - x)^2 + (\eta + z)^2} \]
\[ + \frac{4\eta z(\eta + z)[(z + \eta)^2 + x^2 - ax]}{[(a - x)^2 + (\eta + z)^2]^2} \]
\[ - \frac{4\eta z(\eta + z)[(z + \eta)^2 + x^2 + ax]}{[(a + x)^2 + (\eta + z)^2]^2} \]
\[ + \frac{(\eta - z)[x^2 - ax + (\eta - z)^2]}{(a - x)^2 + (\eta - z)^2} \]
\[ - \frac{(\eta - z)[x^2 + ax + (\eta - z)^2]}{(a + x)^2 + (\eta - z)^2} \]
\[ + \frac{\eta - z}{2} \left\{ \ln \left[ \frac{(a - x)^2 + (\eta - z)^2}{(a - x)^2 + (\eta + z)^2} \right] \right. \]
\[ - \ln \left[ \frac{(a + x)^2 + (\eta - z)^2}{(a + x)^2 + (\eta + z)^2} \right] \]
\[ , \tag{B6} \]

\[ F_{11}^4 = \frac{4\eta(a - x)[(a^2 - 2ax + \eta^2 + x^2)^2 - z^4]}{[(a - x)^2 + (\eta - z)^2][(a - x)^2 + (\eta + z)^2]^2} \]
\[ + \frac{4\eta(a + x)[(a^2 + 2ax + \eta^2 + x^2)^2 - z^4]}{[(a + x)^2 + (\eta - z)^2][(a + x)^2 + (\eta + z)^2]^2} \]
\[ - 2 \left[ \tan^{-1} \left( \frac{a - x}{\eta - z} \right) + \tan^{-1} \left( \frac{a - x}{\eta + z} \right) \tan^{-1} \left( \frac{a + x}{\eta - z} \right) \right. \]
\[ + \left. \tan^{-1} \left( \frac{a + x}{\eta + z} \right) \right] \]
\[ , \tag{B7} \]
\[ E_{11}^+ = \frac{4cz(\eta + z)[(z + \eta)^2 + x^2 - ax]}{[(a - x)^2 + (\eta + z)^2]^2} \]

\[ - \frac{4\eta z(\eta + z)[(z + \eta)^2 + x^2 + ax]}{[(a + x)^2 + (\eta + z)^2]^2} \]

\[ - \frac{11\eta z^2 + 13\eta^2 z + 3\eta x^2 - ax(3\eta + z) + zx^2 + 3\eta^3 + z^3}{(a - x)^2 + (\eta + z)^2} \]

\[ + \frac{11\eta z^2 + 13\eta^2 z + 3\eta x^2 + ax(3\eta + z) + zx^2 + 3\eta^3 + z^3}{(a + x)^2 + (\eta + z)^2} \]

\[ - \frac{(\eta - z)[(\eta - z)^2 + x^2 - ax]}{(a - x)^2 + (\eta - z)^2} \]

\[ + \frac{(\eta - z)[(\eta - z)^2 + x^2 + ax]}{(a + x)^2 + (\eta - z)^2} \]

\[ - 2x \left[ \tan^{-1} \left( \frac{a - x}{\eta - z} \right) + \tan^{-1} \left( \frac{a - x}{\eta + z} \right) + \tan^{-1} \left( \frac{a + x}{\eta - z} \right) \right] \]

\[ + \tan^{-1} \left( \frac{a + x}{\eta + z} \right) - \frac{3(\eta - z)}{2} \ln \left[ \frac{(a - x)^2 + (\eta - z)^2}{(a + x)^2 + (\eta - z)^2} \right] \]

\[ - \frac{5\eta + 3z}{2} \ln \left[ \frac{(a - x)^2 + (\eta + z)^2}{(a + x)^2 + (\eta + z)^2} \right] \]

\[ F_{22}^- = \frac{8\eta z^2(a - x)[(a - x)^2 + z^2 - \eta^2]}{[(a - x)^2 + (\eta - z)^2][(a - x)^2 + (\eta + z)^2]^2} \]

\[ + \frac{8\eta z^2(a + x)[(a + x)^2 + z^2 - \eta^2]}{[(a + x)^2 + (\eta - z)^2][(a + x)^2 + (\eta + z)^2]^2} \]
\[ E_{22}^+ = \frac{7\eta z^2 + 5\eta^2 - \eta x^2 - ax(\eta - z) + zx^2 - \eta^3 + z^3}{(a - x)^2 + (\eta + z)^2} \]

\[ - \frac{7\eta z^2 + 5\eta^2 z - \eta x^2 - ax(\eta - z) + zx^2 - \eta^3 + z^3}{(a + x)^2 + (\eta + z)^2} \]

\[ + \frac{(\eta - z)[(\eta - z)^2 + x^2 - ax]}{(a - x)^2 + (\eta - z)^2} \]

\[ - \frac{(\eta - z)[(\eta - z)^2 + x^2 + ax]}{(a + x)^2 + (\eta - z)^2} \]

\[ - \frac{4\eta z(\eta + z)[(z + \eta)^2 + x^2 - ax]}{[(a - x)^2 + (\eta + z)^2]^2} \]

\[ + \frac{4\eta z(\eta + z)[(z + \eta)^2 + x^2 + ax]}{[(a + x)^2 + (\eta + z)^2]^2} \]

\[ + \frac{\eta - z}{2} \left\{ \ln \left[ \frac{(a - x)^2 + (\eta - z)^2}{(a - x)^2 + (\eta + z)^2} \right] \right. \]

\[ - \ln \left[ \frac{(a + x)^2 + (\eta - z)^2}{(a + x)^2 + (\eta + z)^2} \right] \}

\[ , \ (B10) \]

\[ F_{12}^- = \frac{\eta^2 + 4\eta z + z^2}{(a + x)^2 + (\eta + z)^2} - \frac{\eta^2 + 4\eta z + z^2}{(a - x)^2 + (\eta + z)^2} \]

\[ + \frac{4\eta z(\eta + z)^2}{[(a - x)^2 + (\eta + z)^2]^2} \]

\[ - \frac{1}{2} \left\{ \ln \left[ \frac{(a - x)^2 + (\eta + z)^2}{(a - x)^2 + (\eta - z)^2} \right] - \ln \left[ \frac{(a + x)^2 + (\eta + z)^2}{(a + x)^2 + (\eta - z)^2} \right] \right\} \]

\[ , \ (B11) \]

\[ - \frac{4\eta z(\eta + z)^2}{[(a + x)^2 + (\eta + z)^2]^2} + \frac{(\eta - z)^2}{(a - x)^2 + (\eta - z)^2} \]

\[ - \frac{(\eta - z)^2}{(a + x)^2 + (\eta - z)^2} \]
\[ E_{12} = \frac{2\eta z[(a + x)(\eta + z)^2 - (a - x)^3]}{((a - x)^2 + (\eta + z)^2)^2} \]
\[ + \frac{2\eta z[(a - x)(\eta + z)^2 - (a + x)^3]}{((a + x)^2 + (\eta + z)^2)^2} - \frac{a(z^2 + 4\eta z + \eta^2)}{(a - x)^2 + (\eta + z)^2} \]
\[ - \frac{a(\eta - z)^2}{(a + x)^2 + (\eta - z)^2} \]
\[ + \frac{a(\eta - z)^2}{(a + x)^2 + (\eta - z)^2} \]
\[ - 2(\eta - z) \left[ \tan^{-1} \left( \frac{a - x}{\eta - z} \right) + \tan^{-1} \left( \frac{a + x}{\eta - z} \right) \right] \]
\[ - \frac{x}{2} \left\{ \ln \left[ \frac{(a - x)^2 + (\eta + z)^2}{(a - x)^2 + (\eta - z)^2} \right] - \ln \left[ \frac{(a + x)^2 + (\eta + z)^2}{(a + x)^2 + (\eta - z)^2} \right] \right\} \]
\[ + 2(\eta + z) \left[ \tan^{-1} \left( \frac{a - x}{\eta + z} \right) + \tan^{-1} \left( \frac{a + x}{\eta + z} \right) \right] \]
Appendix C

The surface normal displacement $u(x)$ can be decomposed as follows: (1) the surface displacement $u^\Gamma(x)$ due to subsurface cracks and (2) the surface displacement $u^0(x)$ due to the loading body in contact with a homogeneous half-space.

The surface normal displacement induced by an edge dislocation at $(0, \eta)$ can be written as [162]:

$$u_y = \frac{1}{2\pi(\kappa + 1)} (b^+ U_{yy} + b^+ U_{xy})$$

where

$$U_{yy} = (\kappa + 1) \left( \frac{\pi - 2 \tan^{-1} \frac{x}{\eta}}{\eta} + \frac{2\eta}{r^2} (\kappa - 1) \right),$$

$$U_{xy} = -\frac{2\eta^2}{r^2} (\kappa + 1),$$

$$r^2 = \eta^2 + x^2.$$  \hspace{1cm} (C4)

Using the linear functions to model the dislocation densities, the climb dislocation $\rho^\perp$ and glide dislocation $\rho^\parallel$ can be denoted as $\rho^\perp = c^\perp x + d^\perp$ and $\rho^\parallel = c^\parallel x + d^\parallel$, respectively. Therefore, The normal displacement due to a horizontal crack with length $2a$ centered at $(0, \eta)$ can be obtained by

$$u^\Gamma(x, \eta) = \frac{1}{2\pi(\kappa + 1)} \int_{-a}^{a} \left[ \rho^\perp(x') U_{yy}(x-x', \eta) + \rho^\parallel(x') U_{xy}(x-x', \eta) \right] dx'$$

$$= H^\perp(x, \eta)c^\perp + K^\perp(x, \eta)d^\perp + H^\parallel(x, \eta)c^\parallel + K^\parallel(x, \eta)d^\parallel.$$  \hspace{1cm} (C5)

The expressions for $H^\perp$, $K^\perp$, $H^\parallel$ and $K^\parallel$ can be calculated as follows (according to the works done by Zhou and Wei [29]):
\[ H^{\perp} = \frac{1}{2\pi(\kappa + 1)} \left[ \tan^{-1} \left( \frac{a-x}{\eta} \right) + \tan^{-1} \left( \frac{a+x}{\eta} \right) \right] \left( \kappa a^2 + 3\kappa \eta^2 - \kappa x^2 + a^2 - \eta^2 - x^2 \right) - a \eta \frac{3\kappa - 1}{\pi(\kappa + 1)} - \frac{\kappa \eta x}{\pi(\kappa + 1)} \ln \left( \frac{a^2 - 2ax + x^2 + \eta^2}{a^2 + 2ax + x^2 + \eta^2} \right) , \quad (C6) \]

\[ K^{\perp} = \frac{1}{\pi} \left[ (a-x) \tan^{-1} \left( \frac{a-x}{\eta} \right) + (a+x) \tan^{-1} \left( \frac{a+x}{\eta} \right) \right] + \frac{\kappa \eta}{\pi(\kappa + 1)} \ln \left( \frac{a^2 + 2ax + x^2 + \eta^2}{a^2 - 2ax + x^2 + \eta^2} \right) + a , \quad (C7) \]

\[ H^+ = -\frac{\eta x}{\pi} \left[ \tan^{-1} \left( \frac{a-x}{\eta} \right) + \tan^{-1} \left( \frac{a+x}{\eta} \right) \right] - \frac{\eta^2}{2\pi} \ln \left( \frac{a^2 - 2ax + x^2 + \eta^2}{a^2 + 2ax + x^2 + \eta^2} \right) , \quad (C8) \]

\[ K^+ = -\frac{\eta}{\pi} \left[ \tan^{-1} \left( \frac{(a-x)}{\eta} \right) + \tan^{-1} \left( \frac{(a+x)}{\eta} \right) \right] . \quad (C9) \]

When considering the contact problem with multiple cracks, the surface displacement \( u_a^r \) at the element \([\alpha, 0]\) can be obtained by summing up all the displacement contributions of the edge dislocations in the computational domain:

\[ u_a^r = \sum_{\xi=0}^{N\gamma-1} \sum_{\xi'=0}^{N\gamma'-1} (H^{\perp}_{a-\xi,\xi'} c^{\xi,\xi'}_{\xi'} + K^{\perp}_{a-\xi,\xi'} d^{\xi,\xi'}_{\xi'} + H^+_{a-\xi,\xi'} c^{\xi,\xi'}_{\xi'} + K^+_{a-\xi,\xi'} d^{\xi,\xi'}_{\xi'}) . \quad (C10) \]

The surface normal displacement \( u_a^0 \) at the element \([\alpha, 0]\) due to surface normal pressure and tangential traction can be obtained by

\[ u_a^0 = \sum_{\xi'=0}^{N\gamma'-1} Q^{0}_{a-\xi'} p_{\xi,0} + \sum_{\xi'=0}^{N\gamma'-1} Q^{\xi}_{a-\xi'} f_{\xi,0} , \quad 0 \leq \alpha \leq N\gamma - 1. \quad (C11) \]

The \( Q^{0}_{a-\xi'} \) and \( Q^{\xi}_{a-\xi'} \) are the coefficients relating the normal surface displacement \( u_a^0 \) at the observation point \((x_a, 0)\) to the constant normal pressure \( p_{\xi,0} \) and constant tangential traction \( f_{\xi,0} \) on the discretized surface area centered at \((x_{\xi}, 0)\), respectively.
Appendix D

Based on the previous study of Zhou et al. [14], the elastic-plastic stress field in three-dimensional materials with inhomogeneous inclusions subjected to contact loading can be decomposed into three parts: (1) the stress $\sigma_{\alpha,\beta,\gamma}^1$ due to the contact body, (2) the stress $\sigma_{\alpha,\beta,\gamma}^2$ due to the equivalent plastic strains, and (3) the stress $\sigma_{\alpha,\beta,\gamma}^3$ caused by the equivalent eigenstrains, which used to model the inhomogeneous inclusions according to the EIM. Based on the stress superposition, the total stresses can be expressed as

$$\sigma_{\alpha,\beta,\gamma} = \sigma_{\alpha,\beta,\gamma}^1 + \sigma_{\alpha,\beta,\gamma}^2 + \sigma_{\alpha,\beta,\gamma}^3.$$  \hspace{1cm} (D1)

The contact stress $\sigma_{\alpha,\beta,\gamma}^1$ in a half-space can be caused by the surface pressure $p_{\xi,\zeta}$ and shear traction $f_{\xi,\zeta}$. It can be obtained by

$$\sigma_{\alpha,\beta,\gamma}^1 = \sum_{\xi=0}^{N_x-1} \sum_{\zeta=0}^{N_y-1} M^n_{\alpha-\xi,\beta-\zeta,\gamma} p_{\xi,\zeta} + \sum_{\xi=0}^{N_x-1} \sum_{\zeta=0}^{N_y-1} M^f_{\alpha-\xi,\beta-\zeta,\gamma} f_{\xi,\zeta},$$ \hspace{1cm} (D2)

where $M^n_{\alpha-\xi,\beta-\zeta,\gamma}$ and $M^f_{\alpha-\xi,\beta-\zeta,\gamma}$ are $6 \times 1$ matrix forms of the influence coefficients induced by $p_{\xi,\zeta}$ and $f_{\xi,\zeta}$ on a surface element, respectively.

The stress $\sigma_{\alpha,\beta,\gamma}^2$ induced by the equivalent plastic strains can be calculated by

$$\sigma_{\alpha,\beta,\gamma}^2 = \sum_{\xi=0}^{N_x-1} \sum_{\zeta=0}^{N_y-1} \sum_{\phi=0}^{N_z-1} A_{\alpha-\xi,\beta-\zeta,\gamma-\phi} \varepsilon_{\xi,\zeta,\phi}^{**},$$ \hspace{1cm} (D3)

where $A_{\alpha-\xi,\beta-\zeta,\gamma-\phi}$ is a $6 \times 6$ matrix forms of the influence coefficients which relate the stresses at the observation point $(x_\alpha, y_\beta, z_\gamma)$ in the cuboid $[\alpha, \beta, \gamma]$ to the plastic strain $\varepsilon_{\xi,\zeta,\phi}^{**}$ in the cuboid $[\xi, \zeta, \phi]$. The value of $\varepsilon_{\xi,\zeta,\phi}^{**}$ equals zero when
just the elastic deformation occurred and it would be non-zero when the plastic deformation happened.

The eigenstress $\sigma_{\alpha,\beta,\gamma}^3$ caused by the inhomogeneous inclusions can be obtained by

\[
\sigma_{\alpha,\beta,\gamma}^3 = \sum_{\xi=0}^{N_x-1} \sum_{\zeta=0}^{N_y-1} \sum_{\varphi=0}^{N_z-1} A_{\alpha-\xi,\beta-\zeta,\gamma-\varphi} (\varepsilon_{\xi,\zeta,\varphi}^p + \varepsilon_{\xi,\zeta,\varphi}^*) \tag{D4}
\]

where $\varepsilon_{\xi,\zeta,\varphi}^p$ is the initial eigenstrains and $\varepsilon_{\xi,\zeta,\varphi}^*$ is the equivalent eigenstrains.

Finally, the expression of the total stresses can be obtained by

\[
\sigma_{\alpha,\beta,\gamma} = \sum_{\xi=0}^{N_x-1} \sum_{\zeta=0}^{N_y-1} \sum_{\varphi=0}^{N_z-1} A_{\alpha-\xi,\beta-\zeta,\gamma-\varphi} (\varepsilon_{\xi,\zeta,\varphi}^p + \varepsilon_{\xi,\zeta,\varphi}^*) 
+ \sum_{\xi=0}^{N_x-1} \sum_{\zeta=0}^{N_y-1} \sum_{\varphi=0}^{N_z-1} M_{\alpha-\xi,\beta-\zeta,\gamma-\varphi}^p P_{\xi,\zeta} 
+ \sum_{\xi=0}^{N_x-1} \sum_{\zeta=0}^{N_y-1} \sum_{\varphi=0}^{N_z-1} M_{\alpha-\xi,\beta-\zeta,\gamma-\varphi} f_{\xi,\zeta} \tag{D5}
\]

\[
(0 \leq \alpha \leq N_x - 1, 0 \leq \beta \leq N_y - 10, 0 \leq \gamma \leq N_z - 1)
\]
Appendix E

The linear isotropic hardening law describing the size of the yield surface as a function of the accumulated plastic strain $p$ is given as

$$\sigma = \sigma_Y + \frac{E_t}{1 - E_t/E_S} p$$

(E1)

where $\sigma_Y$ is the initial yield stress, $E_S$ is the Young’s modulus, and $E_t$ is the plastic tangential modulus.

The current study follows the idea of Nelias et al. [35] to calculate the increment of plastic strains. Yielding occurs when the condition $f(p + \Delta p) = 0$ is satisfied in the plastic zone. The actual increment of the accumulated plastic strain $\Delta p$ can be obtained through the Newton-Raphson iterative scheme. The yield function can be expanded approximately as

$$f^{(n+1)} = f^{(n)} + \Delta p^{(n)} f_p^{(n)} = 0$$

(E2)

Between two consecutive iterative steps, the correction of the accumulated plastic strain $\Delta p^{(n)}$ can be expressed as

$$\Delta p^{(n)} = -\frac{f^{(n)}}{f_p^{(n)}} = \frac{f^{(n)}}{g_p^{(n)} - \sigma_{VM,p}^{(n)}}$$

(E3)

All of the related variables are updated as follows:

$$\sigma_{VM}^{(n+1)} = \sigma_{VM}^{(n)} + \sigma_{VM,p}^{(n)} \Delta p^{(n)}$$

$$p^{(n+1)} = p^{(n)} + \Delta p^{(n)}$$

$$g^{(n+1)} = g(p^{(n+1)})$$

(E4)

Here, $p^{(1)}$, $\sigma_{VM}^{(1)}$ and $a_{ij}^{(1)}$ are the initial effective plastic strain, equivalent von Mises stress and Cauchy stress components, respectively. The calculation ends if the convergence condition is satisfied:
Appendix E

\[
\begin{vmatrix}
 f^{(n+1)} \\
g^{(n+1)}
\end{vmatrix} = \left| \frac{\sigma_{VM}^{(n+1)} - g^{(n+1)}}{g^{(n+1)}} \right| < \text{tolerance}
\] (E5)

The steps indicated in Eqs. (E2)-(E4) are repeated until the iteration converges.

According to the plastic flow rule, the estimation of the plastic strain increment is determined:

\[
\Delta \varepsilon_{ij}^p = \left[ p^{(n+1)} - p^{(1)} \right] \frac{3S_{ij}^{(n+1)}}{2\sigma_{VM}^{(n+1)}}
\] (E6)
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