A nonlocal damage model for elasto-plastic materials based on gradient plasticity theory

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A nonlocal damage model for elasto-plastic materials based on gradient plasticity theory

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Doctor of Technical Sciences

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Abstract

Experimental and theoretical studies have shown that size effects in structure deformations and failure become significant as soon as strain gradients are high. For instance as soon as material failure dominates a deformation process, the specimen displays increasingly softening and the finite element computation is significantly affected by the element size. Without considering this effect in the constitutive model one cannot hope a reliable prediction to the ductile material failure process. To give an accurate prediction of the structure integrity and to quantify the material failure process, it is necessary to introduce the strain gradients into constitutive equations. Gradient plasticity models have been discussed extensively in recent years. The mesh-sensitivity in numerical analysis has been successfully eliminated and analytical explanations for size effects were given.

In the present work, a general framework for a nonlocal micromechanical damage model based on the gradient-dependent plasticity theory is presented and its finite element algorithm for finite strains is developed and implemented. In the finite element algorithm, equivalent plastic strain and plastic multiplier have been taken as the unknown variables. Due to the implementation of the Lapacian term, the implicit C¹ shape function is applied for equivalent plastic strain and can be transformed to arbitrary quadrilateral elements. Computational analysis of material failure is consistent to the known size effects. By incorporating the Laplacian of plastic strain into the GTN constitutive relationship, the known mesh-dependence is overcome for the simulation of ductile damage processes and numerical results correlate uniquely with the given material parameters.

In the chapters of applications, we discuss simulations of micro-indentation tests based on the gradient plasticity model. The role of intrinsic material length parameters in the gradient plasticity model is investigated. The computational results confirm that the gradient plasticity model is suitable to simulate micro-indentation tests. It is found that micro-hardness of metallic materials depends significantly on the indentation depth. Variations of micro-hardness are correlated with the intrinsic material length parameters.
The size effect analysis of concrete structures shows that the gradient plasticity model can describe the size effect of load carrying capacity and strain-softening if the size dependence of fracture energy and tensile strength are introduced in a realistic way. The failure mode of concrete changes from ductile to brittle when the size of an element increases.

Finally the micro-mechanical damage model based on gradient-dependent plasticity is applied to the ductile failure of the German reactor pressure vessel steel 20MnMoNi55. Computational simulations of uniaxial smooth and round-notched tensile specimens and notched bending specimens are presented. The different material failure loads in the tensile bars are used to fit the material parameters. It is found that the effects of gradient regulation variations in the smooth tensile specimens are negligible due to small strain gradients. The computational results essentially agree with the experimental data. In notched tensile specimens the strain gradients change local material deformations and damage more significantly. The decreasing of scaled material strength can be predicted by the intrinsic material length scale parameter. By introducing the intrinsic material length scale the material failure is affected by the absolute specimen size. The gradient plasticity provides a new frame for a better assessment of material failure, independently of the finite element mesh design.
Zusammenfassung


Die Untersuchungen zum Grösseneffekt von Betonstrukturen ergaben, dass das Gradienten-Plastizitätsmodell die Grösseneinflüsse von Belastungskapazität und Dehnungsentfestigung gut beschreibt, wenn die Grössenabhängigkeit der Bruchenergie und der Zugfestigkeit realistisch vorgegeben werden. Die Versagensart von Beton ändert sich von duktil zu spröd bei Zunahme der Elementgrösse.

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Chapter 1

Introduction

It is known that conventional continuum mechanics treats mathematical continua, that is, solids of continuum mechanics consist of mathematical points and do not contain micro-structures. It follows that the stress state is determined by the deformation history at this single material point. Although the conventional continuum mechanics is quite sufficient for most applications, there are experimental evidences which indicate that under some specific conditions the material micro-structures must be taken into account in a suitable way.

For ductile materials, in bending of thin nickel beams with the beam thickness ranging from 12.5 to 100 microns, Stolken and Evans [76] observed that plastic work hardening increases with the decrease of thickness of the thin beams. In torsion tests Fleck et al. [28] found that the torque normalized by the twist of a thin wire of copper with a diameter of 12 microns was as high as three times of that in a wire with the diameter of 120 microns. In uniaxial tension the material strength becomes scalable by a geometry factor. Recently, experiments on micro- and nano-indentation hardness tests have been extensively investigated for determining material characteristics in micro-dimension [49], [50], [65], [70]. It has been found that the micro-hardness of materials is significantly higher than the macro-hardness by a factor of two or more in the range from about 50 microns to 1 micron. For quasi-brittle materials, e.g. concrete, the damage development has a strong size effect [13]. For granular materials, e.g. soils and rocks, similar phenomenon can be found in the failure by localization [88]. Generally, it can be concluded the smaller the scale, the stronger will be the solid. All
these observations imply that the inhomogeneity of material's micro-structures may induce the size influence of material response. In fact, all solid materials have substructures or microstructures, e.g. crystal lattice, inclusions, grains and grain clusters. Therefore materials should have some characteristic lengths (the size or distance of substructure). In the frame of classical continuum mechanics theory, there are some models to interpret size effects, e.g., viscoplasticity theory which becomes apparent when the flow stress is strain rate dependent, may be responsible for size effects. Statistical theory plays a prominent role and is widely used to explain size effects especially for brittle fracture and fatigue. Although these classical models have been used spreadly, there is still a necessity to construct non-classical continuum mechanics theories which consider this heterogeneity on a phenomenological level and still treat the material as a continuum.

Recently, material modeling including microstructure characteristics has been extensively discussed. A variety of models incorporating material length scales by nonlocal integral-type or gradient-type formulation has been proposed. Nonlocal integral concepts which involve a finite neighborhood volume integral of a state variable (damage) is used by Cabot and Bazant [62]. The original motivation of this model comes from the problem of localization into shear bands. In recent years, many different nonlocal gradient-type models under different assumptions and considerations were proposed. Menzel and Steinmann [51] suggested the continuum formulation of higher gradient plasticity for single and polycrystals, which incorporates for single crystals second order spatial derivatives of the plastic deformation gradients and for polycrystals fourth order spatial derivatives of the plastic strain into yield condition. Acharya and Bassani [2] developed the gradient theory of crystal plasticity in which the strain gradient effects represent an internal variable acting to increase the current tangent-hardening modulus. Andrieux et al. [8, 40] proposed the nonlocal constitutive models with gradients of internal variables derived from a micro/macro homogenization procedure. All these efforts make the gradient-type approach attractive in modern solid mechanics.

Fleck and Hutchinson [28, 30] considered an 'asymmetric' strain gradient plasticity theory based on the physical concept of geometrically necessary dislocations. In their theory additional high-order strain tensor and the work conjugated moment stress tensor enter
the material model and governing equations. From view point of application the Fleck-Hutchinson strain gradient plasticity theory is similar to Cosserat type continuum which introduces length scale by additional degrees of freedom of deformations. This strain gradient plasticity theory as well as Gao et al. [32] has been successfully used to analyze the size effects of micro-indentation tests, torsion deformation and metal matrix composite [14, 32, 37, 71, 72, 73]. However, no applications are known to localization of deformation and shear banding problems since the Cosserat type continuum has problem in tension dominated applications where rotations are small. The effect of the high-order strain become insignificant within the localization band [24]. Furthermore, it is still open whether or not such models may generate a physical meaningful shear band analysis at strain localization. From the view point of application, the theory may be too weak to overcome the mesh-dependence in finite element simulation due to strain softening.

Aifantis [4] suggested a simple form of plasticity depending on plastic strain gradients which is termed gradient plasticity theory. In this theory, the scalar variable, i.e. the Laplacian of the equivalent plastic strain is included into the usual yield condition and constitutive equation. So the difficulties exhibited by the classical plasticity can be eliminated when the material enters the softening regime. Using the gradient terms, it is possible to determine the shear band width and to perform mesh-dependent finite element calculations. The corresponding gradient coefficients measuring the effect of gradient terms, turned out to relate directly to the internal length scales which characterize the underlying dominant microstructure. The thermodynamical consistence of the gradient plasticity model has been discussed by Valanis [87] and Polizzotto [64]. The finite element implementation of the gradient plasticity has been published by de Borst and co-workers [24, 58] and extended to finite strains by Mikkelsen [52, 53] and Ramaswamy [66] using slightly different interpolation algorithms. Additional work on the finite element implementation of gradient plasticity models can be found by Li and Cescotto [48], Comi [22], Teixeira de Freitas et al. [31] and Oka et al. [57]. Recently this model is implemented into meshless methods by Chen, Wu and Belytschko [20] and finite difference method by Alehossein et al. [7]. Works in [24, 58] showed that the Aifantis model containing only the second order of the plastic strain gradient gave mesh-independent predictions of brittle material failure. On the other hand,
Introduction

This model is successfully used to explain the size effects exhibited by twisted wires and metal matrix composite [97, 6]. Due to the hopeful applications of gradient plasticity, the idea of gradient plasticity is extended to construct a gradient-enhanced damage model by de Borst and co-workers [59, 60, 33] for concrete in which the crack behaviour is brittle and not accompanied by significant plastic deformation. Several gradient plasticity models coupled to phenomenological damage are also discussed by de Borst [26], Svedberg and Runesson [77, 78], respectively.

Failure in ductile metals is characterized by the micro-void nucleation, growth and coalescence mechanism. The Gurson damage model (GTN model) [82, 83, 84], originally introduced by Gurson [35] and later modified by Tvergaard and Needleman, is not derived from purely heuristic arguments but from micromechanical analysis. The yield function of the GTN model accounts for voids in terms of one single internal variable, the void volume fraction or the porosity. This model is popular in materials mechanics community to analyze and to predict failure of ductile metallic materials. However, a well known problem is that strain localization and so material failure are concentrated in the single layer of finite elements, due to involved strain softening in the material failure process, resulting in a zero dissipated energy as the element size becomes vanishingly small. The finite element simulations show an inherent mesh sensitivity in ductile material failure simulations. These observations imply that there is a need for such a micromechanical approach to incorporate the intrinsic material length parameter into the constitutive relation.

Nonlocal forms of the Gurson model in which the delocalization is related to the damage parameter were developed by Leblond [46], Tvergaard and Needleman [86] et al. In these investigations the porosity is treated nonlocally by averaging the actual porosity value in an assumed neighboring region. From numerical point of view, such approach is similar to those to fit a constant element size with the material microstructure [17, 75, 91], in which the size of a cell element is chosen to be representative of the mean spacing between voids. It follows that each cell element contains a single void at the initial volume fraction. Growth and coalescence of the void is related to the stress and strain averaged over the cell element. In comparison with the integration treatment, the cell element method is simpler for finite element computations. However, its application is restricted in small size specimen due to
increasing computational efforts.

Recently, Ramaswamy and Aravas [66] suggested a gradient formulation of the porosity in the Gurson model. In their study, effects of void diffusion, interaction and coalescence have been considered. In their model the first and second derivatives of the porosity enter the evolution equation. Variations of the porosity are controlled by a diffusion equation.

All these approaches assume that the material length scale is only related to damage development. Gradients of the porosity affect material failure process, which is certainly contradictory to the known experimental observation of size effects in plasticity [28].

In the present work, one aim is to derive and formulate the GTN damage constitutive model [35, 83] based on Aifantis gradient plasticity theory under finite strain assumption. A suitable finite element algorithm is formulated. In the nonlocal finite element algorithm the numerical convergence and efficient solution is an important point to verify the gradient plasticity theory. Investigation of numerical convergence speed as well as numerical stability and use of the efficient solution are an important task of the present work. The mesh-independent numerical solution is the basis for the development of a new nonlocal damage model in this work. Furthermore, the aim of the thesis is to formulate not only a pure mathematical model but also physically meaningful constitutive relationship using experimental data. The new algorithm can be applied for a better assessment in the structural integrity analysis. Therefore the model parameters are determined both by the finite element calculation of the cell model in which the meaning of the material microstructure can be identified and by the numerical simulation of the fracture experiments of selected material. This new nonlocal damage model contributes to a better understanding of strain localization and material damage.

The thesis is organized as follows. In chapter 2 the development of gradient plasticity theory is reviewed. The boundary conditions of gradient plasticity for different cases are discussed. In chapter 3 the finite element algorithm for gradient plasticity under finite element assumption is formulated based on the former works of Pamin [58] and Mikkelsen [52, 53]. In this chapter an implicit Hermitian interpolation functions, proposed by Petera and Pittman [61] for equivalent plastic strain, are selected. Then the element can be transformed from
rectangular to arbitrary quadrilateral which is more suitable for finite strain deformation. The shear band analysis is used to verify the interpolation method. Different examples show that the mesh-dependence of shear band is removed and the width of shear band is uniquely determined by the coefficient of Laplacian term.

Chapter 4 derives and formulates the Gurson damage model based on gradient plasticity theory. In this chapter the mixed finite element formulation is implemented with three kinds of nodal degrees of freedom, the displacement, the equivalent plastic strain and plastic multiplier. The variational principle similar to that in chapter 4 is proposed for the constitutive relationship. Due to the nonlinear construction of Gurson constitutive equation and the nonlinear relation between equivalent plastic strain and plastic multiplier, the $C^1$-continuous interpolation for plastic strain is unavoidable. The equivalent plastic strain is interpolated by the implicit Hermitian functions. The plastic multiplier uses the interpolation method suggested by Pinsky [63] and Simo [69]. Numerical examples show that using this element formulation the mesh-dependence of damage localization is removed and the material length scales predicts size effects in material failure.

In chapter 5 the finite element algorithm is applied to investigate the size dependent micro-hardness which has been analyzed and captured by Fleck and Hutchinson's strain gradient theory. The gradient terms in gradient plasticity are investigated and numerical results are compared with the experimental data. The hardness prediction based on gradient plasticity coincides with the known prediction of Nix and Co-workers [56], [50]. In chapter 6 an algorithm similar to the work of Pamin [58] is used and applied to the size effect analysis of quasi-brittle materials.

In chapter 7 the size effect of ductile material is analyzed with the nonlocal damage model. The nonlocal GTN damage model are applied to analyze the size effect of ductile material at room temperature. The smooth and notched tensile specimens are studied. The intrinsic length scale is identified from the computation.

Main assumptions of this work are the static loading and room temperature conditions. Conventional notation is used throughout. Each symbol is defined when it appears at the first time or when it changes its meaning. Boldface symbols denote vectors and tensors. All
vector and tensor component are written with respect to the Cartesian coordinate system. The summation convention is used for repeated indices. A superscript $T$ or $t$ means the transpose of a vector or a tensor. A superposed dot indicates the material time derivative.
Chapter 2

Review of gradient plasticity theory

It is well known that the classical plasticity theories can be roughly divided into two types: deformation theory and flow theory. Deformation theory considers the entire deformation history and relates the total plastic strain to the final stress, while flow theory deals with a succession of infinitesimal increments of distortion in which the instantaneous stress is related to the infinitesimal increment of strain. Generally, flow theory is appropriate to describe plastic deformation involving loading and unloading, while deformation theory is mathematically convenient for proportional loading and suitable for providing insight. In the present dissertation, flow theory is considered into finite element codes and deformation theory is only used for the discussions of boundary conditions and size effects in this chapter.

2.1 The gradient plasticity theory

Classical continuum models suffer from pathological mesh dependence in strain-softening materials. The reason is that in this case the critical condition for localization coincides with the condition for loss of ellipticity of the governing differential equations. The difficulty of mathematical model reflects the absence of internal length scales in the governing equations. As a result, no information pertaining to the way of communication between the various slices of the material was include in the constitutive description, thus no predictions on
Plastic deformations in metals arise from the accumulation of dislocations. From the study of dislocation motions, it is clear that the stress and strain state of a material point is influenced by distortions in its neighborhood, that is, plastic deformations are generally nonlocal. Based on the study of dislocation motion and evolution, it is possible to consider problems at a macroscopic scale by producing suitable relations for the deformation and also understand phenomena occurring at a microscopic level by producing appropriate partial differential equations of diffusion-reaction type for the temporal and spatial evolution of microstructures. Therefore higher order spatial and/or time derivatives has been introduced to address the heterogeneity and deformation patterning during plastic flow [3]. It is known that the resulting nonlinear differential equation can be solved to give the sharp variation of the strain profile inside and outside the shear band region in the case of shear bands analysis. These gradients provide a stabilizing mechanism, make the appropriate partial differential equations describing the material response in the pre-localization regime to be continuously valid and give useful results in the post-localization. As stated by Aifantis [5], the use of higher order strain gradients in the 'softening' deformation regime for obtaining the thickness of shear bands was motivated by the mechanical theory of liquid-vapor interfaces. In the case of shear bands, higher order strain gradients are introduced either into the non-convex expression for the flow stress of plastic materials and the resulting nonlinear differential equation is solved to give the sharp variation of the strain profile inside and outside the shear band region.

The gradient-dependence has first been used in the theory of rigid-plastic material for the analysis of persistent slip band by Aifantis [3, 4] and shear bands in metals by Coleman and Hodgdon [21]. This approach is used as a localization limiter by Belytschko and Lasry [15]. In this chapter, the gradient plasticity theory is reviewed.

The simplest form of gradient plasticity is based on the gradient modification of the expression for the flow stress \( \sigma = \sigma_y(\dot{\varepsilon}^p) \) to include the Laplacian of the equivalent plastic strain, i.e. \( \nabla^2\dot{\varepsilon}^p \).

\[
\sigma_y(\dot{\varepsilon}^p, \nabla^2\dot{\varepsilon}^p) = \sigma_y(\dot{\varepsilon}^p) - g\nabla^2\dot{\varepsilon}^p
\] (2.1)
The gradient plasticity theory

The corresponding form of the yield equation can be written as

\[ \Phi(\bar{\sigma}(\varepsilon^p, \nabla^2\varepsilon^p)) = \phi(\bar{\sigma}(\varepsilon^p)) - g\nabla^2\varepsilon^p, \quad (2.2) \]

where \( \phi(\bar{\sigma}(\varepsilon^p)) \) is the classical J2 yield stress measure, \( \varepsilon^p \) is the equivalent plastic strain and \( g \) is a positive coefficient with the dimension of force. They are expressed as

\[ \phi(\bar{\sigma}(\varepsilon^p)) = \sqrt{S_{ij}S_{ij}/2} \quad (2.3) \]
\[ \varepsilon^p = \sqrt{2\dot{\varepsilon}_{ij}\dot{\varepsilon}_{ij}} \quad (2.4) \]

The flow rule deriving from the yield function (2.2) reads:

\[ \varepsilon_{ij}^p = \lambda \frac{\partial \Phi}{\partial \sigma_{ij}} \quad (2.5) \]

where \( \lambda \) is a plastic multiplier. \( \frac{\partial \Phi}{\partial \sigma_{ij}} = n_{ij} \) defines the direction of the plastic flow. According to the elasto-plastic theory the stress can be expressed as

\[ \dot{\sigma}_{ij} = C^e_{ijkl}(\varepsilon_{kl} - \varepsilon_{kl}^p) \quad (2.6) \]

with the elasticity matrix \( C^e_{ijkl} \). For isotropic solids the elasticity matrix can be simplified into

\[ C^e_{ijkl} = (K - \frac{2}{3}G)I_{ij}I_{kl} + 2GI'_{ijkl} \quad (2.7) \]

where \( K \) and \( G \) are the elastic bulk and shear moduli, respectively. \( I_{ij} \) is the second order identity tensor, and \( I'_{ijkl} \) is the fourth order symmetric identity tensor with Cartesian components \( I'_{kl} = (\delta_{kl}\delta_{ji} + \delta_{ij}\delta_{jk})/2 \), \( \delta_{ij} \) being the Kronecker delta. During plastic flowing, the stress point must remain on the yield surface in the stress space:

\[ \Phi(\bar{\sigma}(\varepsilon^p, \nabla^2\varepsilon^p)) = 0 \quad (2.8) \]

The introduction of the Laplacian of equivalent plastic strain into flow stress and yield function is adopted by several researchers [24, 52, 54, 58, 64, 66, 78] and succeeded in the analysis of strain localization into shear band. However, there is evidence that the first order gradient of plastic strain can not be omitted under some circumstance, e.g., in pure bending test, Richard [68] observed the size effect of yield initiation. If the gradient plasticity theory is used to explain this phenomenon and only the Laplacian of plastic strain is introduced...
into the flow stress, no size effect can be achieved due to $\nabla^2 \varepsilon^p = 0$ in pure bending. For this reason, in the work of size effects analysis by Aifantis [6], the first-order derivative, $|\nabla \varepsilon^p|$, is included. Then flow stress and constitutive equation can be written as

$$
\sigma_y(\varepsilon^p, |\nabla \varepsilon^p|, \nabla^2 \varepsilon^p) = \sigma_y(\varepsilon^p) + g_1 |\nabla \varepsilon^p| - g \nabla^2 \varepsilon^p
$$

for plastic work, the following equations can be written as

$$
\Phi(\sigma_y(\varepsilon^p), |\nabla \varepsilon^p|, \nabla^2 \varepsilon^p)) = \phi(\sigma(\varepsilon^p)) + g_1 |\nabla \varepsilon^p| - g \nabla^2 \varepsilon^p
$$

The Eqn. (2.8) can be expressed as

$$
\frac{\partial \Phi}{\partial \sigma_{ij}} \sigma_{ij} + \frac{\partial \Phi}{\partial \varepsilon^p} \dot{\varepsilon}^p + \frac{\partial \Phi}{\partial |\nabla \varepsilon^p|} |\nabla \dot{\varepsilon}^p| + \frac{\partial \Phi}{\partial \nabla^2 \varepsilon^p} \nabla^2 \dot{\varepsilon}^p = 0,
$$

Where $g_1$ is also a positive coefficient. In this dissertation, we assume that $g_1$ and $g$ can be expressed for ductile materials in the following way

$$
g_1 = \sigma_0 l_1 f_1(\varepsilon^p)
$$

$$
g = \sigma_0 f(\varepsilon^p).
$$

where $\sigma_0$ is the initial yield stress; $l_1$ and $l$ are intrinsic length scale parameters; $f_1(\varepsilon^p)$ and $f(\varepsilon^p)$ are two dimensionless functions of equivalent plastic strain in general.

For Von Mises plasticity, it is known that $\varepsilon^p = \lambda$. Then the consistency condition takes the form:

$$
n_{ij} \dot{\sigma}_{ij} + \frac{\partial \Phi}{\partial \lambda} \dot{\lambda} + \frac{\partial \Phi}{\partial |\nabla \lambda|} |\nabla \dot{\lambda}| + \frac{\partial \Phi}{\partial \nabla^2 \lambda} \nabla^2 \dot{\lambda} = 0.
$$

Eqn. (2.14) is a differential equation for $\lambda$ in contrast to the classical plastic case where $\lambda$ is determined from an algebraic equation. By solving the differential equation and Eqn (2.1-2.8), the gradient plasticity theory can be used to analyze plastic behaviour of materials.

### 2.2 Size effects and strain gradient interpretation

It is well known that the nominal tensile strength of many materials undergoes very clear size effects. This is more evident for disordered materials (e.g., concrete, rocks, ceramics) [19]. Lately it has been experimentally verified that the mechanical behaviour ranges from ductile to brittle when the structural size alone is increased and the material and geometry
size effects and strain gradient interpretation

shape are kept unchanged. As described by Bazant [11], there are six different size effects that may cause the nominal strength to depend on structure size: 1. Boundary layer effect, also known as the wall effect; 2. Diffusion phenomena, such as heat conduction or pore water transfer; 3. Hydration heat or other phenomena associated with chemical reactions; 4. Statistical size effect, which is caused by the randomness of material strength been believed to explain most size effects in concrete structures; 5. Fracture mechanics size effect, due to the release of stored energy of the structure into the fracture front; and 6. Fractal nature of crack surfaces.

In the classical theories based on plasticity or limit analysis, the strength of geometrically similar structures is independent of the structure size. As pointed out in introduction of this dissertation, there are more and more experimental evidences to verify the size effects of nominal strength even for ductile materials due to the fact that current applications in modern technology involve a variety of length scales ranging from a few centimeters down to few nanometers. Therefore classical plasticity theory does not cover all kinds of size effects. However, on the other hand, the interaction between macroscopic and microscopic length scales in the constitutive response and the corresponding interpretation of the associated size effects can be modeled through the introduction of higher order strain gradients in the respective constitutive equations [6].

Due to the introduction of gradient terms into flow stress and yield function, material length scales are included into the coefficients \( g_1 \) and \( g \). If the high order gradients, i.e., Eqn. (2.9) is considered for a priori strain field (deformation theory), different length scales can lead to different stress distribution for the same strain field. One can immediately conclude that the material strength is dependent on the length scales. It means the strain gradients have the potential to interpret the size effects of material strength. In fact, the size effects of material strength using gradient plasticity has been investigated by several researchers [6, 97]. In this section, the application of the gradient plasticity model to investigate the phenomena that are influenced by plastic strain gradients, e.g. bending of thin beams, torsion of thin wires, are reviewed. Details can be found in the work of Aifantis [6].
**Bending of thin beams** In the four-point-bending experiment of mild steel beam of different size, Richard [68] observed that the value of yield initiation (upper yield stress) increases significantly as the specimen size is decreased from the largest to the smallest. The size effect cannot be explained by Aifantis gradient plasticity theory if only the Laplacian of plastic strain is involved due to $\nabla^2 \varepsilon^p = 0$ in pure bending. For this reason, the first order gradient $|\nabla \varepsilon^p|$ plays an important role in the analysis of size effect of thin beams' bending.

A Cartesian reference coordinate system in $(x_1, x_2)$ plane is set and the neutral axis of the beam is assumed to coincide with $x_1$ axis. The curvature of the beam is designated $\kappa$ and the thickness is $2h$. The displacements of the beam are:

$$ u_1 = \kappa x_1 x_2, \quad u_2 = k(x_1^2 + x_2^2)/2 $$  \hspace{1cm} (2.15)

Strains in the Cartesian coordinates, $\varepsilon_{ij}$, the equivalent strain $\bar{\varepsilon}$ under plane strain condition ($\varepsilon_{33} = 0$) and incompressibility condition ($\varepsilon_{kk} = 0$) are given by

$$ \varepsilon_{11} = -\varepsilon_{22} = \kappa x_2, \quad \varepsilon_{12} = 0, \quad \bar{\varepsilon} = \frac{2}{\sqrt{3}} k |x_2| $$  \hspace{1cm} (2.16)

Using gradient deformation theory for the analytical convenience, the form of yield function is:

$$ \dot{\sigma} = f(\bar{\varepsilon}) + g_1 |\nabla \bar{\varepsilon}| - g |\nabla^2 \bar{\varepsilon}| $$  \hspace{1cm} (2.17)

where the equivalent stress $\dot{\sigma}$ and the equivalent plastic strain $\bar{\varepsilon}$ are defined by

$$ \dot{\sigma} = \sqrt{\frac{3}{2} s_{ij} s_{ij}}, \quad \bar{\varepsilon} = \sqrt{\frac{2}{3} \varepsilon_{ij} \varepsilon_{ij}} $$  \hspace{1cm} (2.18)

with $f(\bar{\varepsilon})$ denoting the usual homogeneous flow stress, $g_1 = g_1(\bar{\varepsilon})$ and $g = g(\bar{\varepsilon})$ being the gradient coefficients. The constitutive equation in gradient plasticity is formally identical to the classical plasticity theory

$$ s_{ij} = \frac{2\dot{\sigma}}{3\bar{\varepsilon}} \varepsilon_{ij} $$  \hspace{1cm} (2.19)

where $\dot{\sigma}$ depends on gradients of equivalent plastic strain as defined in (2.17). Then deviatoric stresses of the bending beams can be obtained from Eqn. (2.19), which read

$$ s_{11} = -s_{22} = \frac{\dot{\sigma}}{\sqrt{3} |x_2|}, \quad \sigma_{12} = 0 $$  \hspace{1cm} (2.20)
The stresses can be expressed as

\[ \sigma_{11} = \frac{\bar{\sigma}}{\sqrt{3}} x_2, \quad \sigma_{22} = 0 \]  

(2.21)

and the equivalent stress is

\[ \bar{\sigma} = f(\dot{\varepsilon}) + \frac{2\kappa}{\sqrt{3}} g_1 \]  

(2.22)

The bending moment \( M \) is obtained from the integration over the cross section of the beam as:

\[ M = \int_{-h}^{h} \frac{2}{\sqrt{3}} \bar{\sigma} |x_2| dx_2 = M_0 + \frac{4}{3} h^2 \kappa g_1 \]  

(2.23)

where \( M_0 = \int_{-h}^{h} \frac{2}{\sqrt{3}} f(\dot{\varepsilon}) |x_2| dx_2 \) is the bending moment for classical plasticity theory. From this expression it can be seen that the moment \( M \) is linearly correlated with the curvature and the gradient plasticity coefficient \( g_1 \). Since the deformation is known a priori, the equivalent plastic strain is determined by the deformation field. The increasing length scale do increase the bending strength.

**Torsion of thin wires** The experiments reported by Fleck et al. [29] have been investigated gradient effects in twisting of thin copper wires and predicted that the scaled shear strength increases three times as the wire diameter decreases from 170 to 12 microns. Here the gradient plasticity theory is used to investigate and analyze this phenomenon.

The Cartesian reference system is set such that the \( x_1 \) and \( x_2 \) axes are within the cross section of the wire, while the \( x_3 \) axis coincides with the central axis of the wire. The twist per unit length is designated \( \kappa \) and the radius of the wire is \( a \). The displacement field is known a priori:

\[ u_1 = -\kappa x_1 x_2, \quad u_2 = \kappa x_1 x_2 \]  

(2.24)

The non-vanishing strains and the equivalent strain are given by:

\[ \epsilon_{13} = -\frac{\kappa}{2} x_1, \quad \epsilon_{23} = \frac{\kappa}{2} x_1, \quad \dot{\varepsilon}^p = \frac{1}{\sqrt{3}} \kappa \sqrt{x_1^2 + x_2^2} \]  

(2.25)

The corresponding constitutive equation (2.19) gives non-vanishing deviatoric stresses as

\[ s_{13} = \frac{2\epsilon_{13}}{3\dot{\varepsilon}} \bar{\sigma}, \quad s_{23} = \frac{2\epsilon_{23}}{3\dot{\varepsilon}} \bar{\sigma} \]  

(2.26)
where the equivalent stress equals to

\[ \bar{\sigma} = f(\bar{\varepsilon}) + \frac{\kappa}{\sqrt{3}} (g_1 - \frac{g}{r}) \]  

(2.27)

It is interesting to note that the first gradient term increases the strength while the Laplacian term decreases it. The torque \( T \) can be obtained from the integration over the cross section of the torques induced by the section:

\[ T = \frac{2}{\sqrt{3}} \pi \int_0^a \bar{\sigma} r^2 dr = T_0 + \frac{2a^3 \pi \kappa}{3} \left[ g_1 - \frac{g}{2a} \right] \]  

(2.28)

where \( T_0 \) is the torque obtained by classical plasticity. According to Eqn. (2.28), it is found that if only Laplacian of gradient plastic strain is involved into constitutive equation and flow stress, the torque decreases with coefficient \( g \) increasing. Therefore the small size specimen has lower strength than the big one for the given coefficient \( g \). This is opposite to the observation by Fleck et al. [29]. On the other hand, it is obvious that in torsion of a solid wire the parameter \( g \) must be a plastic strain-dependent parameter, otherwise the stress at \( r = 0 \) will be infinite. For this reason, Aifantis changed his gradient plasticity model slightly for torsion test and tried to fit the experiment data [6].

### 2.3 Boundary conditions for gradient plasticity

In the construction of the variational principle for gradient plasticity theory, Mühlhaus and Aifantis [54] assumed that at the elastic-plastic boundary \( \nabla \lambda = 0 \). This condition is widely adopted [24, 52, 54, 58, 64, 66, 78, 16]. Using the nonlocal thermodynamic theoretical framework, the consistence of gradient plasticity theory are discussed by Polizzotto [64], Valanis [87], Lorentz and Andrieux [47] and Svedberg et al. [77]. They concluded that the boundary condition of \( \nabla \lambda \), derived from energetic approach, is tangential to the boundary surface enclosing any finite region where plastic deformation mechanism takes place, and need not be stated a priori. It is true for simple shear and strain localization. Unfortunately, in other cases, i.e., pure bending, pure torsion and void growth, the boundary condition can not be fulfilled due to the a priori deformation field. In fact, the boundary conditions of gradient plasticity is still open and need more careful discussions. In this section, these boundary conditions are reviewed and discussed.
Simple shear  An infinite strip over the domain \((-H \leq x_2 \leq H, -\infty \leq x_1 \leq \infty\) with a one dimensional distribution of displacement \(u_1(x_2)\) and an associated distribution of shear strain \(\gamma(x_2) = \partial u_1 / \partial x_2\) is considered. The shear stress \(\tau\) is constant in the field. In classical plasticity theory, the shear strain in the field is also constant, while in gradient plasticity the shear strain field is related to the gradients of shear strain and generally not constant. The governing second order differential equation for this shear strain can be obtained from gradient plasticity theory:

\[ \tau = G \gamma + g_1 |\gamma| - g_2 \gamma_{x_2} \]  

(2.29)

Where \(G\) is shear modulus. Eqn. (2.29) have analytical solutions. In order to obtain a unique solution for \(\gamma(x_2)\), an additional boundary condition is needed. For instance, \(\gamma_2 = 0\) and \(\gamma = 0\) at \(x_2 = \pm H\) can be assumed. These boundary conditions are definitely the conclusions from thermodynamic analysis [64].

One dimensional strain localization  A uniaxial bar of length \(L\) with the ends \(x = -L/2\) and \(x = L/2\) subjected to the displacements \(-u/2\) and \(u/2\) respectively, is taken into account. The stress \(\sigma > 0\) is constant throughout the bar. The bar is assumed elastic-softening plastic:

\[ \sigma = \sigma_y + h \varepsilon^p(x) \]  

(2.30)

where \(h\) is the softening modulus, assumed to be negative and constant. In order to get the unique width of localization band, only Laplacian of equivalent plastic strain are introduced into flow stress and yield equation. The governing differential equation is:

\[ \sigma = \sigma_y + h \varepsilon^p - g \varepsilon_{x_2}^p \]  

(2.31)

De Borst and Mülhaus suggest \(g = -hl^2\) where \(l\) is the intrinsic length scale related to the gradient coefficient \(g\). By solving Eqn. (2.31) with the boundary conditions \(\varepsilon^p = 0\) and \(\varepsilon_{x_2}^p = 0\) for \(x = \pm w\), the plastic strain field in the bar is:

\[ \varepsilon^p = \frac{\sigma - \sigma_y}{h} \left[ 1 - \frac{\cos(x/l)}{\cos(w/2l)} \right] \]  

(2.32)

The relation between \(l\) and \(w\) can be given from the condition \(d\varepsilon^p / dw = 0\), which leads to the equation:

\[ \cos(w/2l) = 1 \]  

(2.33)
The equation has the smallest non-trivial solution \( w = 2\pi l \). This solution verifies again that the natural boundary condition must be enforced.

Based on the analysis of the two examples, it can be known that using gradient plasticity and considering the natural boundary conditions, the new plastic deformation field obtained by gradient plasticity, is different from that solved by conventional plasticity theory.

**Spherical voids.** An isolated spherical void of radius \( a \) is subjected to uniform remote spherically symmetric loading specified by \( \sigma^\infty \) in an infinite, incompressible solid. The spherical coordinate system \((r, \theta, \phi)\) is originated at the void center. From the incompressibility of materials follows the non-vanishing displacement

\[
\mathbf{u}_r = \frac{a^2}{r^2} \mathbf{u}_0
\]

where \( \mathbf{u}_0 \) is the displacement on the void surface. The non-vanishing strains and the effective strain are given by

\[
\epsilon_{rr} = -2\epsilon_{\theta\theta} = -2\epsilon_{\phi\phi} = -\frac{2a^2}{r^3} \mathbf{u}_0, \quad \bar{\epsilon} = \frac{2a^2}{r^3} \mathbf{u}_0
\]

From the constitutive equation (2.19), the deviatoric stress are expressed as

\[
\sigma_{rr} = -2\sigma_{\theta\theta} = -2\sigma_{\phi\phi} = \frac{2}{3} \bar{\sigma}
\]

with

\[
\bar{\sigma} = f(\bar{\epsilon}) + \frac{6a^2 \mathbf{u}_0}{r^4} - \frac{24a \mathbf{u}_0}{r^5}
\]

The stress component \( \sigma_{rr} \) can be determined by integrating the equilibrium equation in the polar coordinates

\[
\sigma_{rr} = -\int_a^r \frac{2\sigma_{rr} - \sigma_{\theta\theta} - \sigma_{\phi\phi}}{r} dr = 2\int_a^r \frac{\bar{\sigma}}{r} dr
\]

where it assumes traction-free on the void surface. From the equation above the remote applied symmetric stress can be calculated as

\[
\sigma^\infty = 2 \int_a^\infty \frac{\bar{\sigma}}{r} dr = \sigma_0^\infty + \frac{3\mathbf{u}_0}{a^2} - \frac{48\mathbf{u}_0}{5a^3}
\]

where \( \sigma_0^\infty = 2 \int_a^\infty \frac{f(\bar{\epsilon})}{r} dr \) is the remote stress calculated by classical plasticity.
Cylindrical voids. An isolated cylindrical void of initial radius \( a \) in an infinite, incompressible solid is considered. The solid is subjected to uniform remote cylindrically symmetric loading specified by \( \sigma^\infty \) under plane strain conditions. The cylindrical coordinate system \((r, \theta, z)\) is originated at the void center. The non-vanishing displacement, strain and the effective strain are given by

\[
\begin{align*}
\epsilon_r &= \frac{a}{r} u_0, \\
\epsilon_{rr} &= -\epsilon_{\theta\theta} = -\frac{a}{r^2} u_0, \\
\bar{\epsilon} &= \frac{2a}{\sqrt{3}r^2} u_0
\end{align*}
\] (2.40)

where \( u_0 \) is the displacement on the void surface. From the constitutive equation (2.19), the deviatoric stress are expressed as

\[
\begin{align*}
\sigma_{rr} &= \sigma_{\theta\theta} = -\frac{1}{\sqrt{3} \bar{\sigma}}
\end{align*}
\] (2.41)

with \( \bar{\sigma} = f(\bar{\epsilon}) + g_1 \frac{4u_0}{\sqrt{3}r^2} - g_2 \frac{8u_0}{3a^3} \). The stress component \( \sigma_{rr} \) can be determined from the equilibrium equation in the polar coordinates

\[
\sigma_{rr} = -\int_a^r \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} dr = \frac{2}{\sqrt{3}} \int_a^r \bar{\sigma} \frac{dr}{r}
\] (2.42)

where it assumes traction-free on the void surface. The remote applied symmetric stress can be calculated as

\[
\sigma^\infty = \int_a^r \sigma_{rr} \frac{dr}{r} = \sigma^\infty_0 + g_1 \frac{8u_0}{9a^2} - g_2 \frac{4u_0}{3a^3}
\] (2.43)

where \( \sigma^\infty_0 = \int_a^r \frac{f(\bar{\epsilon})}{r} dr \) is the remote stress calculated by classical plasticity.

Discussions According to Eqns. (2.39) and (2.43) it can be found that the Laplacian terms of equivalent strain are negative in the expression. If only Laplacian term is involved in flow stress, the strength decreases with the increasing of coefficient \( g \). This issue has raised some doubts in the work of Zhu and Zbib [97]. They applied the gradient plasticity theory only using Laplacian of equivalent plastic strain into flow stress to investigate the size effect of strain gradient in metal matrix composite. In their study, the variation of plastic dissipation within a volume \( V \) is:

\[
\delta W = \frac{1}{V} \int_V \delta w dV = \frac{1}{V} \int_V \bar{\sigma} \delta \bar{\epsilon} dV = \frac{1}{V} \int_V \left[ f(\bar{\epsilon}) - g \nabla^2 \bar{\epsilon} \right] \delta \bar{\epsilon} dV
\] (2.44)

By means of the divergence theorem

\[
\int_V \nabla^2 \bar{\epsilon} \delta \bar{\epsilon} dV = \int_V \nabla \bar{\epsilon} \cdot \nabla \delta \bar{\epsilon} dV - \int_S \delta \bar{\epsilon} \nabla \bar{\epsilon} \cdot \mathbf{n} dS
\] (2.45)
and the boundary condition $\nabla \varepsilon \cdot n = 0$ on the surface which is derived from the thermodynamical analysis, the variation of plastic work becomes

$$\delta W = \frac{1}{V} \int_V [\delta w_0 + g \nabla \varepsilon \cdot \nabla \delta \varepsilon] dV$$

(2.46)

where $\delta w_0 = f(\varepsilon) \delta \varepsilon$ is the variation of plastic work by classical plasticity. Thus the total strain energy for the gradient dependent material can be expressed as

$$W = \frac{1}{V} \int_V [w_0 + g \nabla \varepsilon \cdot \nabla \varepsilon] dV$$

(2.47)

According to Eqn. (2.47) the strength of gradient dependent material increases with the increasing of coefficient $g$. In this case, the strain field is determined by incompressibility of material and no strain gradient boundary condition can be enforced on the boundary. Under these two special circumstances, the boundary condition is not satisfied and the gradient term acts as a destabilizing manner. As mentioned before, only using the first gradient term can not overcome the mesh-dependence in numerical analysis due to strain softening. Therefore the Laplacian term is necessary. More investigations are necessary to analyze whether or not the boundary condition can be fulfilled.

In experiments of metal matrix composite, Barlow and Hansen [10] found that experimentally measured strain gradient is almost an order of magnitude smaller than a classical theory's predictions. It implies that new deformation field is given by considering the gradient effects of strain field. Referred to the discussion of strain localization and the case when the deformation field is not known a priori, it is found that using the gradient plasticity as well as the boundary condition $\nabla \varepsilon \cdot n = 0$ on the boundary surface can give the new solution for plastic strain field. So it is assumed in the dissertation that when the strain field around a void is not known a priori (except the special cases above), the boundary condition $\nabla \varepsilon \cdot n = 0$ is enforced on the boundary of the void. In this way the gradient plasticity theory with the boundary condition $\nabla \varepsilon \cdot n = 0$ is used to investigate effects of void growth.

Although the problems and arguments still exist in the boundary conditions of gradient plasticity theory, $\nabla \lambda = 0$ are enforced on the boundary in the computational model of this dissertation. More discussions on boundary condition of computational model due to the interpolation method are investigated in the following chapters.
Chapter 3

Computational gradient plasticity on finite strains

3.1 Conventional non-linear finite element methods

For problems in materials mechanics when no analytical solution exists, an approximate solution for displacements, deformations, stresses, forces and possibly other state variables can be found by numerical methods. The exact solution of such a problem requires that both force and moment equilibrium are maintained at all times over any arbitrary volume of the body. The displacement finite element is based on approximation of this equilibrium requirement by replacing it with a weaker requirement. Equilibrium must be maintained in an average sense over a finite number of divisions of the body volume. Let \( V \) denote a volume occupied by a part of the body in current configuration, and \( S \) be the surface bounding this volume. Let the surface traction at any point on \( S \) be the force \( \mathbf{t} \) per unit of current area, and the body force at any point within the volume of material under consideration be \( \mathbf{b} \) per unit of current volume. The weak form of translational equilibrium is as follows:

\[
\int_{V} \left[ \frac{\partial}{\partial \mathbf{x}} \cdot \sigma + \mathbf{b} \right] \cdot \delta \mathbf{v} \, dV = 0. \tag{3.1}
\]

Note that \( \sigma = \sigma^{T} \) and \( \mathbf{t} = \mathbf{n} \cdot \sigma \) where \( \sigma \) is the 'true' stress at a point, i.e. the Cauchy stress, \( \mathbf{v} \) is the velocity at a point and \( \mathbf{n} \) is the outward normal vector of the boundary. The
virtual work statement is expressed as:

$$\int \sigma : \frac{\partial \delta \mathbf{v}}{\partial \mathbf{x}} dV = \int_S \mathbf{t} \cdot \delta \mathbf{v} dS + \int_V \mathbf{b} \cdot \delta \mathbf{v} dV. \quad (3.2)$$

Introducing the expression \( \delta \mathbf{D} = \text{sym}(\delta \mathbf{L}) \) where \( \delta \mathbf{L} = \frac{\partial \delta \mathbf{v}}{\partial \mathbf{x}} \), the virtual work equation in classical form gives:

$$\int \sigma : \delta \mathbf{D} dV = \int_S \mathbf{t} \cdot \delta \mathbf{v} dS + \int_V \mathbf{b} \cdot \delta \mathbf{v} dV. \quad (3.3)$$

\( \mathbf{D} \) is the rate of deformation and \( \mathbf{x} \) are the spatial coordinates of the point. Generally the strain is defined as the integral of the rate of deformation. This integration is nontrivial, particularly in the general case where the principal axes of strain rotate during deformation. In this paper, the finite element for gradient plasticity is implemented into ABAQUS by its user element interface. Therefore we follow the strain definition in ABAQUS where the total strain is constructed by integrating the strain rate approximately over the increment by the central difference algorithm and the strain at the start of the increment must also be rotated to consider the rigid body rotation occurring in this increment when the strain components are referred to a fixed coordinate basis. This integration method, suggested by Hughes and Winget [38], defines the integration of a tensor associated with the material behaviour as

$$\mathbf{a}_{t+\Delta t} = \Delta \mathbf{R} \cdot \mathbf{a}_t \cdot \Delta \mathbf{R}^T + \Delta \mathbf{\alpha}(\Delta \mathbf{\epsilon}), \quad (3.4)$$

where \( \mathbf{a} \) is a tensor; \( \Delta \mathbf{\alpha} \) is the increment in the tensor associated with the constitutive behaviour, and therefore dependent on the strain increment, \( \Delta \mathbf{\epsilon} \), defined by the central difference formula as

$$\Delta \mathbf{\epsilon} = \text{sym}\left(\frac{\partial \Delta \mathbf{u}}{\partial \mathbf{x}_{t+\Delta t/2}}\right) \quad (3.5)$$

where \( \mathbf{x}_{t+\Delta t/2} = (1/2)(\mathbf{x}_t + \mathbf{x}_{t+\Delta t}) \); \( \Delta \mathbf{R} \) is the increment in rotation, defined as

$$\Delta \mathbf{R} = (\mathbf{I} - \frac{1}{2}\Delta \mathbf{\omega})^{-1} \cdot (\mathbf{I} + \frac{1}{2}\Delta \mathbf{\omega}), \quad (3.6)$$

where \( \Delta \mathbf{\omega} \) is the central difference integration of the rate of spin

$$\Delta \mathbf{\omega} = \text{asym}\left(\frac{\partial \Delta \mathbf{u}}{\partial \mathbf{x}_{t+\Delta t/2}}\right)$$

and \( \mathbf{I} \) is the second order identity tensor. The definition of strain tensor is

$$\mathbf{\epsilon}_{t+\Delta t} = \Delta \mathbf{R} \cdot \mathbf{\epsilon}_t \cdot \Delta \mathbf{R}^T + \Delta \mathbf{\epsilon} \quad (3.7)$$
and the stress is integrated as:

\[ \sigma_{t+\Delta t} = \Delta R \cdot \sigma_t \cdot \Delta R^T + \Delta \tilde{\sigma}(\Delta \epsilon), \]  

(3.8)

where \( \Delta \tilde{\sigma}(\Delta \epsilon) \) is the stress increment caused by the straining of the material during this time increment. The subscripts \( t \) and \( t + \Delta t \) refer to the beginning and the end of the increment, respectively. For the Newton algorithm, the Jacobian of the equilibrium equations is required. To develop the Jacobian, Eqn. (3.3) is transformed by taking the time differentiation. It gives

\[ \int_V d\sigma \cdot \delta D dV - \int_S dt^T \cdot \delta v dS - \int_V db^T \cdot \delta v dV = 0, \]  

(3.9)

where \( d\sigma \) and \( \sigma \) are evaluated at the end of the increment. Using the integration definition above, it can be shown that

\[ d\sigma_{t+\Delta t} = d\Delta R \cdot \Delta R^T \cdot (\sigma_{t+\Delta t} - C : \Delta \epsilon) + (\sigma_{t+\Delta t} - C : \Delta \epsilon) \cdot \Delta R \cdot d\Delta R^T + C : d\Delta \epsilon \]  

(3.10)

where \( C \) is the Jacobian matrix of the constitutive model (elasto-plasticity matrix in this thesis). Then Eqn. (3.9) is approximated as suggested by ABAQUS by using co-rotational stress rate:

\[ d\sigma_{t+\Delta t} = dR \cdot \sigma_{t+\Delta t} - \sigma_{t+\Delta t} \cdot dR^T + C : dD, \]  

(3.11)

which yields the Jacobian

\[ \int_V \delta D : C : dD - \frac{1}{2} \sigma : \delta(2D \cdot D - \frac{\partial \sigma^T}{\partial x} \cdot \frac{\partial \sigma}{\partial x})dV. \]  

(3.12)

Experience with practice suggests that this approximation of Jacobian provides an acceptable rate of convergence in most applications [1]. In displacement finite element methods, the displacement field is interpolated by:

\[ u = [N]^T \{u^N\} \]  

(3.13)

where \([N]\) are interpolation functions and \([u^N]\) are nodal displacement vector. The virtual field, \( \delta v \), also have the same spatial form

\[ \delta v = [N]^T \{\delta v^N\}. \]  

(3.14)
Then the strain field and virtual strain are expressed as

$$D_{dt} = d\varepsilon = [B]^T \{du_N\}, \quad \delta D = \delta \varepsilon = [B]^T \{\delta v^N\}. \quad (3.15)$$

Substituting these expressions into Eqn. (3.12), we obtain the stiffness matrix:

$$[K] = \int_V [B]^T [C] [B] dv + \int_V ([N_k]^j_T \sigma_{ij} [N_k]_j - 2[B_{ki}]^T \sigma_{ij}[B_{kj}]) dV. \quad (3.16)$$

Here $[B]$ is the strain-displacement relation matrix. Load matrix can be written as

$$\{\mathcal{P}\} = \int_V [N]^T \{b\} dv + \int_S [N]^T \{f\} dV. \quad (3.17)$$

Using the expression (3.16) and (3.17), the Newton iteration form of the classical non-linear finite element equation can be obtained.

### 3.2 Variational formulation for gradient plasticity

Let $V^p$ denote the plastic part volume of the body and $S^p$ be the so-called elastic-plastic boundary surface. As suggested by Mülhaus and Aifantis [54], the generalized variational formulation for gradient plasticity is formulated as

$$\Pi(\dot{\varepsilon}, \dot{\varepsilon}, \delta u, \delta \lambda) = \int_V (\nabla \sigma + \dot{b}) \delta u dV + \int_S \dot{f} \delta u dS + \int_{V^p} \Phi(\sigma(\varepsilon^p), |\nabla \varepsilon^p|, \nabla^2 \varepsilon^p) \delta \lambda dV + \int_{S^p} \frac{\partial \varepsilon^p}{\partial n} \delta \lambda dS. \quad (3.18)$$

The solution is obtained as soon as the generalized variational expression $\Pi$ reaches a stationary point with respect to arbitrary small changes of $(\dot{\varepsilon}, \dot{\lambda})$. Note that for many applications, $\varepsilon^p = \alpha \lambda$ and $\alpha$ is a positive constant. It follows two basic weak form equations as

$$\int_{V^p} \delta (n : \dot{\varepsilon} + \frac{\partial \Phi}{\partial \lambda}) + \frac{\partial \Phi}{\partial |\nabla \lambda|} |\nabla \dot{\lambda}| + \frac{\partial \Phi}{\partial \nabla^2 \lambda} \nabla^2 \dot{\lambda}) dV = - \int_V \delta \lambda \Phi^0(\sigma(\varepsilon^p), |\nabla \varepsilon^p|, \nabla^2 \varepsilon^p)) dV; \quad (3.19)$$

$$\int_V \delta \varepsilon : \dot{\sigma} dV = - \int_V \delta \varepsilon : \sigma^0 dV + \int_V \dot{b} \delta u dV + \int_S \dot{f} \delta u dV \quad (3.20)$$

where $\sigma^0$ and $\Phi^0(\sigma(\varepsilon^p), |\nabla \varepsilon^p|, \nabla^2 \varepsilon^p)$ denote the solution of the previous incremental step and $(\dot{})$ means the material derivative of the corresponding field variable. Considering the finite strain assumption, the Jaumann (co-rotational) stress rate which is suitable for constitutive relationship, can be defined as

$$\dot{\sigma} = \dot{R} : \varepsilon - \sigma \cdot \dot{R} + \sigma^*, \quad (3.21)$$
where $\dot{\sigma}$ is the material derivative of stress tensor and $\sigma^*$ is defined as $\sigma^* = C : \dot{\epsilon}$. The equation (3.20) can be written as

$$
\int_V \delta \sigma : C : D - \frac{1}{2} \sigma : \delta (2 \mathbf{D} \cdot D - \frac{\partial \mathbf{v}^T}{\partial \mathbf{x}} \cdot \frac{\partial \mathbf{v}}{\partial \mathbf{x}}) dV = - \int_V \delta \dot{\epsilon}_{ij} \sigma_{ij} dV + \int_V \mathbf{b} \delta \mathbf{u} dV + \int_S \delta \mathbf{u} dV.
$$

The equations (3.19) and (3.22) build the fundamental for the finite element method. To solve the integral equations above a discretization method must be used to turn the partial differential equations into algebraic equations.

### 3.3 Implicit Hermite interpolation method for equivalent plastic strain

Due to the higher order differentiation of the displacement in Eqn. (3.19, 3.22), the conventional finite element technique based on the $C^0$ interpolation [94] can not be applied. A robust computational algorithm is essential for validation and application of such complex constitutive model.

Ramswamy and Aravas [66] introduced the $C^0$ element by using the Gauss theorem in integration. Such formulation assumes a vanishing normal derivative of the plastic strain at all boundaries, $\partial \lambda / \partial n = 0$. The $C^0$ element formulation is attractive for general robust finite element computation. Such algorithm is, however, only useful for the original gradient plasticity model by Aifantis [4] as in Equation (2.2). As soon as the gradient terms are nonlinear in the constitutive equation, i.e., Gurson constitutive equation (will be discussed in chapter 4), the $C^0$ formulation is not applicable.

Pamin [58] designed series of elements for the gradient plasticity model. The most reliable type is the element with the 8-nodal serendipity interpolation of displacement and 4-nodal Hermitian interpolation of plastic strain with $2 \times 2$ Gaussian point integration. Mikkelsen [52, 53] extended this element type to finite strain assumption and simulated necking of uniaxial tension tests of ductile metallic materials. Due to the explicit Hermitian shape function which is introduced to satisfy requirements of a $C^1$ continuity, the element is
Figure 3.1: The finite element introduced in the present work.

constrained to be rectangular. This results in that the finite element computation may fail to converge if the element strongly distorts.

In the present work we are designing an implicit $C^1$ continuous interpolation function for complex gradient plasticity model. For this purpose the method suggested by Petera and Pittman [61] is adopted, which will be extensively discussed in the following paragraphs.

Let $\varepsilon^p(\xi, \eta) = \varepsilon^p(x(\xi, \eta), y(\xi, \eta))$, where $(\xi, \eta)$ are local reference coordinates and $(x, y)$ are global coordinates. In local coordinate system

$$\varepsilon^p = \mathbf{H}(\xi, \eta)^T \cdot \mathbf{Y}_l, \quad (3.23)$$

where $\mathbf{H}(\xi, \eta)$ is Hermitian shape function in local coordinates and

$$\mathbf{Y}_l = [\ldots; \varepsilon^p, \varepsilon^p_{,\xi}, \varepsilon^p_{,\eta}, \varepsilon^p_{,\xi\eta}, \ldots]^T = [\ldots; \varepsilon^p, \frac{\partial \varepsilon^p}{\partial \xi}, \frac{\partial \varepsilon^p}{\partial \eta}, \frac{\partial^2 \varepsilon^p}{\partial \xi \partial \eta}; \ldots]^T \quad (I = 1, 2, 3, 4) \quad (3.24)$$

denotes the unknown variables as shown in Fig 3.1. $\mathbf{Y}_l$ represents the vector of nodal degrees of freedom for the plastic strain field in local coordinates. The derivatives of $\varepsilon^p$ can be obtained by

$$\varepsilon^p_{,\xi} = \mathbf{H}^T_{,\xi} \cdot \mathbf{Y}_l \quad (3.25)$$

$$\varepsilon^p_{,\eta} = \mathbf{H}^T_{,\eta} \cdot \mathbf{Y}_l \quad (3.26)$$

$$\varepsilon^p_{,\xi\xi} = \mathbf{H}^T_{,\xi\xi} \cdot \mathbf{Y}_l \quad (3.27)$$
Implicit Hermite interpolation method

\[ \varepsilon^p_{,\eta} = \begin{bmatrix} \mathbf{H}^T_{,\eta} \cdot \mathbf{Y}_l \end{bmatrix} \]  
\[ \varepsilon^p_{,\xi} = \begin{bmatrix} \mathbf{H}^T_{,\xi} \cdot \mathbf{Y}_l \end{bmatrix} \]  

The gradient vector of \( \varepsilon^p \) and the Laplacian of \( \mathbf{sp} \) are given by

\[ \nabla \varepsilon^p(\xi, \eta) = \begin{bmatrix} \mathbf{Q}^T \cdot \mathbf{Y}_l \end{bmatrix} \]  
\[ \nabla^2 \varepsilon^p(\xi, \eta) = \begin{bmatrix} \mathbf{P}^T \cdot \mathbf{Y}_l \end{bmatrix} \]  

where \( \mathbf{Q} \) and \( \mathbf{P} \) are derivatives of shape function \( \mathbf{H}^T \) in local coordinate system \((\xi, \eta)\). To obtain \( C^1 \) continuity in the global coordinate system we must transfer all field variables into the \((x, y)\) system. We define

\[ \mathbf{Y}_g = [\ldots; \varepsilon^p_{x,1}, \varepsilon^p_{y,1}, \varepsilon^p_{,\xi,1}, \ldots]^T \quad (I = 1, 2, 3, 4) \]  

as the vector of nodal degrees of freedom in global coordinates. Note that second-order mixed derivative is not transformed according to Petera and Pittman [61]. It turns out that the 4th degree of freedom, \( \varepsilon^p_{,\eta,1} \), is not related to global coordinate system, although this degree of freedom is necessary to make the plastic strain field \( C^1 \) continuous [61]. The field variables are formally expressed as

\[ \mathbf{Y}_l = \mathbf{T} \cdot \mathbf{Y}_g \]  

with

\[ \mathbf{T} = \begin{bmatrix} \vdots & \vdots & \ddots & \ddots & \vdots \\ \vdots & 1 & 0 & 0 & 0 \\ \vdots & 0 & x_{,\eta 1} & y_{,\xi 1} & 0 \\ \vdots & 0 & x_{,\xi 1} & y_{,\eta 1} & 0 \\ \vdots & 0 & 0 & 0 & 1 \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{bmatrix} \quad (I=1, 2, 3, 4; \text{dimension}=16) \]  

After lengthy mathematical manipulations we obtain the interpolation formula in the global system and the Laplacian of plastic strain as

\[ \varepsilon^p(x, y) = \begin{bmatrix} \mathbf{H}^T \cdot \mathbf{Y}_g \end{bmatrix} \]  
\[ \nabla \varepsilon^p(x, y) = \begin{bmatrix} \mathbf{Q}^T \cdot \mathbf{Y}_g \end{bmatrix} \]  
\[ \nabla^2 \varepsilon^p(x, y) = \begin{bmatrix} \mathbf{P}^T \cdot \mathbf{Y}_g \end{bmatrix} \]
The expressions of the interpolation function vector are:

\[ H^T = \bar{H}^T \cdot T \]  \hspace{1cm} (3.38)
\[ Q^T = J \cdot \bar{Q}^T \cdot T \]  \hspace{1cm} (3.39)
\[ P^T = \bar{P}_{1i} + \bar{P}_{2i} \quad (i=1, \, 2, \ldots, 16) \]  \hspace{1cm} (3.40)
\[ \bar{P}^T = R_D \cdot \bar{Q}^T \cdot T + R_B \cdot \bar{P} \cdot T \]  \hspace{1cm} (3.41)

where

\[ J = \begin{bmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \eta}{\partial x} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} \end{bmatrix} \] \hspace{1cm} (3.42)
\[ R_D = \begin{bmatrix} \frac{\partial^2 \xi}{\partial x^2} & \frac{\partial^2 \eta}{\partial y^2} \\ \frac{\partial^2 \xi}{\partial y^2} & \frac{\partial^2 \eta}{\partial x^2} \end{bmatrix} \] \hspace{1cm} (3.43)
\[ R_B = \begin{bmatrix} \left( \frac{\partial \xi}{\partial x} \right)^2 & 2 \left( \frac{\partial \xi}{\partial x} \frac{\partial \eta}{\partial x} \right) & \left( \frac{\partial \eta}{\partial x} \right)^2 \\ \left( \frac{\partial \eta}{\partial y} \right)^2 & 2 \left( \frac{\partial \xi}{\partial y} \frac{\partial \eta}{\partial y} \right) & \left( \frac{\partial \eta}{\partial y} \right)^2 \\ \frac{\partial^2 R_1}{\partial \xi^2} & \ldots & \frac{\partial^2 R_{16}}{\partial \xi^2} \\ \frac{\partial^2 R_1}{\partial \eta^2} & \ldots & \frac{\partial^2 R_{16}}{\partial \eta^2} \end{bmatrix} \] \hspace{1cm} (3.44)
\[ \bar{P} = \begin{bmatrix} \frac{\partial^2 R_1}{\partial \xi^2} & \ldots & \frac{\partial^2 R_{16}}{\partial \xi^2} \\ \frac{\partial^2 R_1}{\partial \eta^2} & \ldots & \frac{\partial^2 R_{16}}{\partial \eta^2} \end{bmatrix} \] \hspace{1cm} (3.45)

To avoid discontinuity in the derivatives of \( x \) and \( y \) with respect to \( \xi \) and \( \eta \), care must be taken in the design of the mesh topology. It means that the adjacent element should have the same local co-ordinate system [61]. For mathematical prove of such formulation as well as details of such interpolation the reader is referred to work of Petera and Pittman [61].

Under finite strain assumptions the Laplacian should be calculated under current configuration. As shown by Mikkelsen [52, 53], an exact evaluation of the Laplacian of plastic strain needs the second derivative of displacement. This makes the \( C^0 \) interpolation for displacement field insufficient. In our study, increments of \( \nabla^2 \varepsilon^p \) as well as \( \Delta (\nabla^2 \varepsilon^p) \) are calculated incrementally in current configuration. Since Laplacian is a scalar, we add all increments...
3.4. Calculation of the tangent stiffness matrix

of $\nabla^2 \varepsilon^p$ and define it as the total Laplacian under current configuration. Such accumulation is accurate under the small rotation conditions. Therefore the $C^1$-continuous interpolation for displacement is avoided.

3.4 Calculation of the tangent stiffness matrix

In Eqns. (3.19) and (3.20/3.22), there appear first order derivatives of the displacements and second order derivatives of plastic strain. Therefore the discretization procedure for the displacement field $u$ requires $C^0$-continuous interpolation functions $N$ and for the equivalent plastic strain $\varepsilon^p$ $C^1$-continuous interpolation functions $H$.

In this work 8-nodal serendipity interpolation functions for displacement field is applied. Generally, the effective plastic strain is a function of plastic multiplier $\lambda$. In this chapter, we limit our interest to the yield functions for which we can write that

$$\dot{\varepsilon}^p = \alpha \dot{\lambda} \quad (3.46)$$

with $\alpha$ constant and positive. For the Von-Mises yield function, we know $\dot{\varepsilon}^p = \dot{\lambda}$. Then the plastic multiplier (effective plastic strain) needs a $C^1$-continuous shape function. At the integration points $d\lambda$, $\nabla d\lambda$ and $\nabla^2 d\lambda$ can be expressed as

$$d\lambda = H^T \cdot d\Lambda \quad (3.47)$$
$$\nabla d\lambda = Q^T \cdot d\Lambda \quad (3.48)$$
$$\nabla^2 d\lambda = P^T \cdot d\Lambda \quad (3.49)$$

where $d\Lambda = d\Upsilon_g$ is the nodal degrees of freedom of effective plastic strain since $d\lambda = d\varepsilon^p$.

In the elasto-plastic continuum we define:

$$d\sigma = C^e (d\varepsilon - d\varepsilon^p) = C^e (d\varepsilon - d\lambda \frac{\partial \Phi}{\partial \sigma}). \quad (3.50)$$

In one increment of finite element solution the stress is defined as:

$$\sigma_{t+\Delta t} = \Delta R^T \sigma_t \Delta R + C^e (\Delta \varepsilon - \Delta \lambda \frac{\partial \Phi}{\partial \sigma}) = \sigma_{t+\Delta t} - \Delta \lambda C^e \frac{\partial \Phi}{\partial \sigma}, \quad (3.51)$$
where $C^e$ is the elastic matrix. For isotropic solids the elasticity matrix can be simplified into

$$
C^e_{ijkl} = (K - \frac{2}{3}G)I_{ij}I_{kl} + 2GI'_{ijkl}
$$

(3.52)

where $K$ and $G$ are the elastic bulk and shear moduli, respectively. $I_{ij}$ is the second order identity tensor, and $I'_{ijkl}$ is the fourth order symmetric identity tensor with Cartesian components $I'_{ijkl} = (I_{ik}I_{jl} + I_{il}I_{jk})/2$. Then the material derivative of Eqn. (3.51) is:

$$
d\sigma = C^e d\epsilon - d\lambda C^e \frac{\partial \Phi}{\partial \sigma} - \Delta \lambda C^e \frac{\partial^2 \Phi}{\partial \sigma^2} d\sigma.
$$

(3.53)

Eqn. (3.53) can be written as

$$
d\sigma = C (d\epsilon - d\lambda \frac{\partial \Phi}{\partial \sigma})
$$

(3.54)

where

$$
C = [(C^e)^{-1} + \Delta \lambda \frac{\partial^2 \Phi}{\partial \sigma^2} d\sigma]^{-1}.
$$

(3.55)

Substituting Eqn. (3.15), (3.35), (3.47), (3.48), (3.49) and (3.55) into the variational functions (3.19) and (3.22) and noting $\frac{\partial \Phi}{\partial \sigma} = n$ and $\frac{\partial \Phi}{\partial \lambda} = h_p$, the two basic equations for finite element formulation are obtained

$$
\int_{V_p} \left[ -Hn^T C B d\epsilon + [(h_p + n^T C n) H H^T + g_1 H Q^T - g H P^T] d\lambda dV = \int_{V_p} \Phi(\lambda, |\nabla \lambda|, \nabla^2 \lambda) H dV,
\right.
$$

$$
\left. \int_{V} [(B^T C B + \tilde{G}^T \sigma \tilde{G}) d\epsilon - B^T C n H^T d\lambda] dV = \int_{V} B^T \sigma_0 dV + \int_{V} N^T b dV + \int_{S} N^T f dV. \right)
$$

(3.56)

In plane strain and axisymmetric assumptions, the matrix $\tilde{G}$ and $\tilde{\sigma}$ are written as

$$
\tilde{\sigma} = \begin{bmatrix}
-\sigma_{11} & -\sigma_{12} & 0 & 0 \\
-\sigma_{12} & -\frac{1}{2}(\sigma_{11} + \sigma_{22}) & -\frac{1}{2}(\sigma_{11} + \sigma_{22}) & 0 \\
0 & -\frac{1}{2}(\sigma_{11} + \sigma_{22}) & -\frac{1}{2}(\sigma_{11} + \sigma_{22}) & -\sigma_{12} \\
0 & 0 & -\sigma_{12} & -\sigma_{11}
\end{bmatrix}
$$

(3.58)
Calculation of the tangent stiffness matrix

\[
\mathbf{G} = \begin{bmatrix}
\cdots & \frac{\partial N_i}{\partial x} & 0 & \cdots \\
\cdots & 0 & \frac{\partial N_i}{\partial x} & \cdots \\
\cdots & \frac{\partial N_i}{\partial y} & 0 & \cdots \\
\cdots & 0 & \frac{\partial N_i}{\partial y} & \cdots \\
\end{bmatrix}
\]

Then we obtain the following set of algebraic equations:

\[
\begin{bmatrix}
\mathbf{K}_{uu} & \mathbf{K}_{u\lambda} \\
\mathbf{K}_{\lambda u} & \mathbf{K}_{\lambda\lambda}
\end{bmatrix}
\begin{bmatrix}
\text{du} \\
\text{d}\lambda
\end{bmatrix}
= \begin{bmatrix}
\mathbf{R}_{\text{load}} \\
\mathbf{f}_{\lambda}
\end{bmatrix},
\]

where

\[
\mathbf{K}_{uu} = \int_V (\mathbf{B}^T \mathbf{C} \mathbf{B} + \mathbf{G}^T \mathbf{G}) dV
\]
\[
\mathbf{K}_{u\lambda} = \int_V \mathbf{B}^T \mathbf{C} \mathbf{n} \mathbf{H}^T dV
\]
\[
\mathbf{K}_{\lambda u} = \int_V -\mathbf{H} \mathbf{n} \mathbf{C} \mathbf{B} dV
\]
\[
\mathbf{K}_{\lambda\lambda} = \int_V (\mathbf{h}_p + \mathbf{n}^T \mathbf{C} \mathbf{n}) \mathbf{H} \mathbf{H}^T + \mathbf{g}_1 \mathbf{H} \mathbf{Q}^T - \mathbf{g} \mathbf{H} \mathbf{P}^T dV
\]
\[
\mathbf{R}_{\text{load}} = -\int_V \mathbf{B}^T \mathbf{\sigma}_0 dV + \int_V \mathbf{N}^T \mathbf{b} dV + \int_S \mathbf{N}^T \mathbf{f} dV
\]
\[
\mathbf{f}_{\lambda} = \int_{V_P} \Phi(\lambda, |\nabla\lambda|, \nabla^2\lambda) \mathbf{H} dV.
\]

The set of Equations (3.58) governs the element behaviour during plastic flow. If all elements are elastic, as suggested by Pamin [58], the vector \( \mathbf{n} \) and \( \mathbf{f}_{\lambda} \) are set to zero. Therefore \( \mathbf{K}_{u\lambda} = \mathbf{K}_{\lambda u} = 0 \) and \( \mathbf{K}_{\lambda\lambda} \) is determined as

\[
\mathbf{K}_{\lambda\lambda} = \sum_{ip=1}^{4} E \mathbf{H}_{ip} \mathbf{H}^T_{ip} V_{ip},
\]

where \( E \) is the Young's modulus and \( V_{ip} \) is a volume contribution of an integration point. If plastic elements appear in the structure, then in elastic elements adjacent to the plastic zone we get \( \mathbf{f}_{\lambda} = 0 \) and non-zero \( d\lambda \) from Eqn. (3.60). Referred to Pamin [58], The 8-nodal \( C^1 \) continuous finite elements have the capacity that the yield strength \( \sigma_y = \bar{\sigma} - g \nabla^2\lambda \) (\( g_1 = 0 \)) is reduced and new elastic elements enter the plastic regime.
3.5 Numerical integration of the constitutive equations

In a finite element method the solution is achieved incrementally with the integration of the governing equations. In a time interval $[t_n, t_{n+1}]$, the stress at $t_{n+1}$, $\sigma_{n+1}$, is calculated as

$$\sigma_{n+1} = \Delta R^T \cdot \sigma_n \cdot \Delta R + C^e \cdot (\Delta \epsilon - \Delta \epsilon^p) = \sigma_{n+1}^e - C^e \cdot \Delta \epsilon^p,$$

(3.62)

where $\sigma_n$ is the known stress state of the previous step, $\Delta \epsilon$ is the known strain increment and $\Delta R$ is the rotation tensor. $\sigma_{n+1}^e = \Delta R^T \cdot \sigma_n \cdot \Delta R + C^e \cdot \Delta \epsilon$ is the elastic trial stress.

In this thesis 8-nodal serendipity interpolation functions for displacement field is applied. Generally the effective plastic strain is a function of plastic multiplier $\lambda$. In this Chapter, we limit our interest to the yield functions for which we can write that

$$\dot{\epsilon} = \alpha \lambda,$$

(3.63)

with $\alpha$ constant and positive. For the Von-Mises yield function, we know $\dot{\epsilon} = \dot{\lambda}$. Then the plastic multiplier (effective plastic strain) needs $C^1$-continuous shape function. For each integration point we know

$$\Delta \lambda = H^T \cdot \Delta \Lambda,$$

(3.64)

$$\nabla \Delta \lambda = Q^T \cdot \Delta \Lambda,$$

(3.65)

$$\nabla^2 \Delta \lambda = P^T \cdot \Delta \Lambda.$$

(3.66)

Then we can get:

$$\lambda_{n+1} = \lambda_n + \Delta \lambda,$$

(3.67)

$$\nabla \lambda_{n+1} = \nabla \lambda_n + \nabla \Delta \lambda,$$

(3.68)

$$\nabla^2 \lambda_{n+1} = \nabla^2 \lambda_n + \nabla^2 \Delta \lambda.$$

(3.69)

For Von-Mises condition, under plane strain or axisymmetric assumptions, it is known

$$n_{n+1} = n_{n+1}^p = \frac{\partial \Phi}{\partial \sigma_{n+1}^e}.$$

Therefore whether the integration point is elastic or plastic in the increment can be judged:

IF $\Phi(\sigma_{n+1}^e, \lambda_{n+1}, |\nabla \lambda_{n+1}|, \nabla^2 \lambda_{n+1}) \geq 0$, 


3.6 Loading/Unloading conditions

In the process of plastic loading and unloading, the Kuhn-Tucher conditions

\[ \lambda \geq 0; \quad \Phi(\varepsilon^p, |\nabla \varepsilon^p|, \nabla^2 \varepsilon^p) \leq 0; \quad \dot{\lambda} \Phi(\varepsilon^p, |\nabla \varepsilon^p|, \nabla^2 \varepsilon^p) = 0 \]  

must be fulfilled. Since the yield condition is enforced globally by integration, difficulty may arise, if the value of the yield function has different signs at the integration points within an element. The respective contributions to residual force \( f_\lambda \) get averaged due to the weak form. However, the 8-nodal \( C^1 \) continuous finite elements have the characteristics that when the global residual vectors, \( \int_\Omega H^T \Phi(\varepsilon^p, \nabla^2 \varepsilon^p) dv \) converge to zero, the value, \( \Phi(\varepsilon^p, \nabla^2 \varepsilon^p) \) at all plastic Gauss points, converge to zero too. If \( \Phi < 0 \), the Gauss point is elastic and \( \lambda \) is forced to zero. Hence the Kuhn-Tucher conditions (3.70) can still be fulfilled at all Gauss points.

3.7 Discussions on boundary conditions

Since the Laplacian of plastic strain is included into the basic governing equations, the additional boundary conditions for plastic strain should be studied. As mentioned in chapter 2, Mühlhaus and Aifantis suggested \( \frac{\partial \varepsilon^p}{\partial n} = 0 \) on the boundary of the plastic-elastic domain in the variational principle. For \( C^1 \) element, this condition is not enough to avoid the singularity of the stiffness matrix. It is useful to examine the rank of submatrices \( K_{uu} \) and \( K_{\lambda \lambda} \) to determine the number of integration points and extra boundary conditions sufficient to avoid spurious modes for both the displacement and plastic strain fields. The matrix \( K_{\lambda \lambda} \) should have at most as many zero eigenvalues as the available boundary conditions for the plastic multiplier (effective plastic strain) field can remove, while it has a number of non-zero eigenvalues equal to the number of integration points (matrix \( HH^T \) has only one non-zero
It should also be taken into account, that a higher-order integration scheme and too many additional boundary conditions for $\lambda$ may lead to an overconstrained plastic flow problem and have a negative influence on the accuracy of finite element predictions. Since the yield condition may be conceived as a differential constraint to the equilibrium condition of a nonlinear solid, we realize that the number of constraints for the plastic multiplier (effective plastic strain) field must be limited, otherwise the solution will be inaccurate or will lock. A proper constraint ratio between the displacement and $\lambda$ degrees of freedom should be preserved.

Pamin [58] suggested that the conditions $\frac{\partial \varepsilon^p}{\partial n} = 0$ and $\frac{\partial^2 \varepsilon^p}{\partial x \partial y} = 0$ on the whole boundary of the specimen supply exactly the required number of constraints. The boundary condition of the mixed derivative of $\varepsilon^p$ is unavoidable. In this dissertation, we assume $\frac{\partial^2 \varepsilon^p}{\partial x \partial n} = 0$ on the whole boundary of the specimen. The correct rank of the stiffness matrix is realized. However the physical meaning of the boundary condition $\frac{\partial^2 \varepsilon^p}{\partial y \partial n} = 0$ still need more discussions.

### 3.8 Mesh sensitivity analysis

#### 3.8.1 Verification of the Hermite interpolation for gradient plasticity

To examine the feasibility of the implicit Hermitian interpolation for the equivalent plastic strains, we consider a tension-dominated specimen with a central circular hole (Fig. 3.2), in which strain localization into shear band takes place at the onset of strain softening. The radius of the hole is $R = 0.1B$. Furthermore, the dimension of the specimen is characterized by $H/B = 2$. Three different meshes with 125, 500 and 825 elements, respectively, are used. The specimen is only loaded at the upper edge by a given uniform vertical displacement. The gradient-dependent von Mises yield condition are taken. Plane strain conditions and infinitesimal deformation assumptions are applied. Elastic modulus is set to $E = 300\sigma_0$. Poisson’s ratio is $\nu = 0.3$. The stress-strain relation is assumed bi-linear characterized by a
Mesh sensitivity analysis

Figure 3.2: Finite element meshes for a specimen with a centered hole. Due to symmetry only a quarter of the specimen is discretised. To study mesh-dependence the meshes contain 125, 500 and 825 elements, respectively. The specimen is loaded only at the upper edge.

negative tangent coefficient $h_p$, that is,

$$\bar{\sigma} = \sigma_0 + h_p \bar{\varepsilon}^p$$

with $h_p = -0.9 \sigma_0$. The material contains strain-softening as soon as it gets plasticity. The yield stress is $\sigma_y = \bar{\sigma} - g \nabla^2 \bar{\varepsilon}^p = \sigma_0 + h_p \bar{\varepsilon}^p - \sigma_0 l^2 \nabla^2 \bar{\varepsilon}^p$. The material length parameter is set to $l = \sqrt{0.002B}$ and $l = \sqrt{0.004B}$, respectively. For $C^1$ elements, the extra boundary conditions for $\bar{\varepsilon}^p$ ($\bar{\varepsilon}^p_{\eta n} = 0$ and $\partial \bar{\varepsilon}^p / \partial n = 0$) are introduced on the whole circumference of the specimen. The material length $l_1 = 0$ is assumed for strain-softening shear band analysis.

The overall stress-strain diagram for the three fine element meshes is plotted in Fig. 3.3. It shows, without gradient influence, that the specimen discretised with the finer element mesh loses strength more quickly than that with the coarser mesh. Setting the material length parameter differs from zero, we can see the mesh-dependence is removed and different meshes give numerically the same strength curve. The material strength is controlled by material parameters, such as $l$, not affected by the element size.

Figure 3.4 shows plastic strain distribution cross the shear band with material length parameter $l = \sqrt{0.002B}$ and $\sqrt{0.004B}$, respectively. The principal strain contour distributions are shown in Figure 3.5. It is clear that the width of the shear band is determined by $l$, as discussed by Pamin [58]. At the center of the shear band, where intense shearing occurs,
Figure 3.3: Overall stress-strain curves for the center-holed specimen with three different FE meshes. The computations are conducted using gradient plasticity without damage. The material length parameter $l = 0, \sqrt{0.002}B$ and $\sqrt{0.004}B$, respectively.

Figure 3.4: Plastic strain distributions along a line perpendicular to the shear band for the center-holed specimen. Three different meshes are used. The overall strain is defined as $\epsilon_{yy} = \Delta H/H = 0.05$. (a) $l = \sqrt{0.002}B$; (b) $l = \sqrt{0.004}B$;
Mesh sensitivity analysis

Figure 3.5: Effects of the element size on principal strain distributions in the center-holed specimen \((\varepsilon_f = 0.1 - 1.0)\) with \(l = \sqrt{0.004B}\)

the \(\nabla \varepsilon_p\) becomes negative, thus the gradient term will arise the flow stress at the center of the shear band. The shear band width is uniquely correlated by the \(l\) value.

3.8.2 Effect of the hole's shape

To show the shear band is determined uniquely by the intrinsic material length, we consider similar tension-dominated specimen but with a central rectangular hole. The length and width of the hole is \(a = 0.1B\). Two different rectangular meshes with 403 and 1020 elements respectively, are used. The same geometry, load and material conditions are used here compared to that in the above subsection. One fourth of the specimen is discretised and shown in Figure 3.6. Since all elements in the meshes are rectangular, the implicit Hermite interpolation method is coincide with the explicit interpolation method used by Pamin et al. Figure 3.7 shows plastic strain distribution cross the shear band with material length \(l = \sqrt{0.002B}\) and \(\sqrt{0.004B}\) respectively. It is proved again that the width of the shear band is determined by \(l\) and mesh dependence is removed by the introduction of material length \(l\). In Figure 3.8 we compared the width of shear band with different central hole. It is found that the width of the shear band is not affected by the shape of holes and the geometry imperfection, but determined uniquely by the material length \(l\). Therefore the intrinsic material length \(l\), acts as a material constant in strain-softening gradient plasticity model. The gradient plasticity model can keep the mesh-objectivity for strain-softening problem.
Figure 3.6: Finite element meshes for a specimen with a centered hole. Due to symmetry only a quarter of the specimen is discretised. To study mesh-dependence the meshes contain 403, 1020 elements, respectively. The specimen is loaded only at the upper edge.

Figure 3.7: Plastic strain distributions along a line perpendicular to the shear band for the center-holed specimen. Two different meshes are used. The overall strain is defined as $\epsilon_{yy} = \Delta H / H = 0.02$. (a) $l = \sqrt{0.002B}$; (b) $l = \sqrt{0.004B}$;
Figure 3.8: Plastic strain distributions along a line perpendicular to the shear band for the center-holed specimen. Two different shapes of hole are used. The overall strain is defined as $\varepsilon_{yy} = \Delta H/H = 0.02$. (a) $l = \sqrt{0.002B}$ ; (b) $l = \sqrt{0.004B}$ ;

With the present example we confirm that the numerical results using different interpolation methods coincide with the known prediction by de Borst and Co. [24, 58]. The interpolation technique is suitable to analyze material failure process using arbitrary element shapes. The gradient plasticity model can provide mesh-independent results for shear band analysis and the width of shear band can be determined by the intrinsic material length $l$ in gradient plasticity theory.
Chapter 4

Nonlocal GTN damage model based on gradient plasticity

All engineering metals and alloys contain inclusions and second-phase particles. In the course of plastic deformation by either debonding or cracking, micro-voids nucleate and grow till a localized internal necking of the intervoid matrix occurs. After a micro-void has nucleated in a plastically deforming matrix it undergoes a volumetric growth and shape change. It can be assumed that the voids are sufficiently far apart so that there is no initial interaction between their local stress and strain fields. Therefore it is possible to develop a model for the early stages of growth in terms of a single void in an infinite plastic solid [17, 18].

4.1 The GTN damage model

For a metal containing a dilute concentration of voids, based on a rigid-plastic upper bound solution for spherically symmetric deformations of a single void, Gurson [35] proposed the following yield condition which was modified by Tvergaard and Needleman [84]:

$$\Phi(q, p, f, \sigma_y) = \frac{q^2}{\sigma_y^2} + 2q_1 f \cosh\left(\frac{3q_2 p}{2\sigma_y}\right) - (1 + q_1 f^2) = 0,$$

(4.1)

where

$$S = pI + \sigma$$

(4.2)
is the deviatoric part of the macroscopic Cauchy stress tensor $\sigma$,

$$ q = \sqrt{\frac{2}{3} S : S } $$  \hspace{1cm} (4.3) $$

is the Mises stress,

$$ p = -\frac{1}{3} \sigma : I $$  \hspace{1cm} (4.4) $$

is the hydrostatic pressure, $f$ is the volume fraction of the voids in the material (porosity), and $\sigma_y(\varepsilon^p)$ is the yield stress of the fully dense matrix material as a function of $\varepsilon^p$, the equivalent plastic strain in the matrix. The constants $q_1$ and $q_2$ were introduced by Tvergaard [84] to bring predictions of the model into closer agreement with full numerical analysis of a periodic array of voids. One can recover the original GTN model by setting $q_1 = q_2 = 1$.

The porous metal plasticity model is intended for use with mildly voided metals. Even though the matrix material is assumed to be plastically incompressible, the plastic behaviour of the bulk material is pressure-dependent, due to the presence of voids. It is noting that $f = 0$ implies that the material is fully dense, and the Gurson yield condition reduces to that of Von Mises; $f = 1$ implies that the material is full of voids, and has no stress carrying capacity. In compression the porous material 'hardens' due to closing of the voids, and in tension it 'softens' due to growth and nucleation of the voids.

Based on the assumption of the plastic flow normality, the macroscopic plastic strain increment is evaluated from

$$ d\varepsilon^p = d\lambda \frac{\partial \Phi}{\partial \sigma}. $$  \hspace{1cm} (4.5) $$

where $d\lambda$ is the non-negative plastic flow multiplier.

The change in volume fraction of voids is caused by both the growth of existing voids and the nucleation of voids. Thus, the evolution equation for the void volume fraction is written as

$$ df = df_{growth} + df_{nucleation}. $$  \hspace{1cm} (4.6) $$

The void growth is described by

$$ df_{growth} = (1 - f) d\varepsilon^p : I, $$  \hspace{1cm} (4.7) $$
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where $\mathbf{I}$ is the second order unit tensor. A strain-controlled nucleation law suggested by Chu and Needleman [23] is

$$\text{d}f_{\text{nucleation}} = \mathcal{A} \text{d}\varepsilon^p,$$

(4.8)

The parameter $\mathcal{A}$ is chosen so that the nucleation strain follows a normal distribution with mean value $\varepsilon_N$ and standard deviation $S_N$. $\mathcal{A}$ can be expressed as:

$$\mathcal{A} = \frac{f_N}{S_N \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{\varepsilon^p - \varepsilon_N}{S_N} \right)^2 \right].$$

(4.9)

where $f_N$ is the volume fraction of void nucleating. Voids are nucleated only in tension. In this thesis the nucleation term is not taken into account if the stress state is compressive.

It is assumed that the microscopic equivalent plastic strain $\varepsilon^p$ varies according to the equivalent plastic work expression,

$$(1 - f)\sigma_y \text{d}\varepsilon^p = \sigma : \text{d}\varepsilon^p = \sigma : \frac{\partial \Phi}{\partial \sigma} \text{d}\lambda$$

(4.10)

The matrix material is assumed to satisfy the von Mises yield condition and the hardening of the matrix material is described by $\sigma_y = \sigma_y(\varepsilon^p)$.

4.2 The GTN damage model coupled to gradient plasticity

In the GTN model one only considers that the material failure process is modeled by nucleation, growth and coalescence of the micro voids. The conventional constitutive relation, which is originally suitable for the macroscopic analysis, is assumed to be valid for the matrix material in microscopic scale. It is an obvious shortcoming in this model [39].

Nonlocal forms of the GTN model in which the delocalization is related to the damage parameter were developed by Leblond [46], Tvergaard and Needleman [86] et al. In their work the porosity is treated nonlocally by averaging the actual porosity value in an assumed neighboring region. Ramaswamy and Aravas [66] suggested a gradient treatment of the porosity of the GTN model. In their study, effects of void diffusion, interaction and coalescence have been considered. The first and second derivatives of the porosity enter the
evolution equation. Variations of the porosity are controlled by a diffusion equation. All these efforts are assuming that the material length is only related to damage development which may be certainly contradictory to the known experimental observation of size effects in plasticity.

Due to existence of voids, the strain field of the porous material is inhomogeneous. In the microscopic level the strain concentrates around the voids. According to recent knowledge, the matrix at microscopic level may have significantly different features from that at the macroscopic cases. Discussions about intrinsic material length make it necessary to introduce a material length into constitutive equation of the matrix. From the view point of gradient plasticity the strain variations may significantly change the matrix strength. In this work, we postulate the matrix strength depending on the strain field. The gradient plasticity is introduced into the matrix material to consider the micromechanisms by voids. In the frame of gradient plasticity, the yield condition is expressed as

\[ \Phi(q, p, f, \sigma_y) = \frac{q^2}{\sigma_y^2(\varepsilon^p, \nabla^2 \varepsilon^p)} + 2q_1 f \cosh\left(\frac{3q_2 p}{2\sigma_y(\varepsilon^p, \nabla^2 \varepsilon^p)}\right) - (1 + q_1^2 f^2) = 0. \]  

In the equation above the actual stress of the matrix, \(\sigma_y(\varepsilon^p, \nabla^2 \varepsilon^p)\), is a function of gradients of plastic strains, represented by \(\nabla^2 \varepsilon^p\). The first order strain gradient \(|\nabla \varepsilon^p|\) is omitted here since only using \(|\nabla \varepsilon^p|\) can not avoid the mesh dependence during damage evolution. If material failure is accompanied with high plastic strain gradients, e.g. near a crack tip, the matrix will be strengthened locally to prevent strain localization. Such consideration is consistent to known experimental observations \[28\].

### 4.3 Governing equations for finite element method

In gradient plasticity theory we have two governing equations which have been introduced in chapter 3, i.e.,

\[ \int_V \delta \lambda (\mathbf{n}^T \dot{\mathbf{\sigma}} - h_p \dot{\varepsilon}^p + g \nabla^2 \varepsilon^p) dV = 0, \]  

\[ \int_V \delta \mathbf{u}^T (\nabla \dot{\mathbf{\sigma}}) dV = 0. \]
which are valid for the damage model by substituting the new yield function (4.11). Due to the complicated constitutive relation between the plastic multiplier $\lambda$ and effective plastic strain $\varepsilon^p$ in equation (4.10), we have to discretise Eqn. (4.10) as the third basic governing equation for the finite element formulation,

$$
\int_V \delta \varepsilon^p [(1-f)\sigma_y \dot{\varepsilon}^p - \boldsymbol{\sigma} : \frac{\partial \Phi}{\partial \boldsymbol{\sigma}} \dot{\lambda}] \, dv = 0. \tag{4.14}
$$

With these three equations, we can design the finite element method for the nonlocal micromechanical damage model coupled to gradient plasticity.

### 4.3.1 Interpolation functions

The basic unknown in the equations (4.12), (4.13) and (4.14) are the displacement vector $u$, the equivalent plastic strain $\varepsilon^p$ as well as the plastic multiplier $\lambda$. The integral expressions will be converted into algebraic equations by using suitable interpolation functions. We take the following interpolations for the field variables

$$
u(x) = [N(x)]u_{node}, \tag{4.15}$$

$$\lambda(x) = [N_1(x)]\lambda_{\text{internal}}, \tag{4.16}$$

$$\varepsilon^p(x) = [H(x)]\varepsilon_{\text{node}}, \tag{4.17}$$

where $[N(x)]$ is the standard 8-nodal serendipity interpolation function for displacement, $[H(x)]$ is the $C^1$-continuous implicit Hermitian interpolation function for plastic strain since the Laplacian of effective plastic strain, $\nabla^2\varepsilon^p$, is introduced into constitutive relationship. $[N_1(x)]$ is the interpolation function for the plastic multiplier. As suggested by Pinsky [63] and Simo[69], the field of $\lambda(x)$ is only to be $L^2(\Omega)$ and discontinuous across the element boundaries. That means the vector $\lambda_{\text{internal}}$ is an internal degree of freedom vector for each individual element. The interpolation function $[N_1(x)]$ is defined as

$$
[N_1(x)] = [h_1(x_j), h_2(x_j), h_3(x_j), h_4(x_j)] \tag{4.18}
$$

where

$$
h_i(x_j) = \begin{cases} 
0 & \text{if } i \neq j \\
1 & \text{if } i = j. 
\end{cases} \tag{4.19}
$$
and \( x_j = (x(\xi_j, \eta_j), y(\xi_j, \eta_j)) \) are Gauss points in global coordinates. In the dissertation the element takes 2 × 2 Gauss point integration. Equations (4.19) may be thought of as defining an orthogonal discontinuous element basis function which assumes a value of 0 or 1 over the quadrants of the bi-unit square domain of the isoparametric coordinates. So using Equation (4.19), the internal vector \( \Lambda_{\text{internal}} \) denotes the value of \( \lambda \) on the 4 Gauss points of each element. Then the three governing equations can be written as

\[
\int_v \mathbf{B}^T \mathbf{d}\sigma + \mathbf{\sigma} \cdot [\mathbf{B}^T \mathbf{B} - \left( \frac{\partial \mathbf{N}}{\partial x} \right)^T \frac{\partial \mathbf{N}}{\partial x}] \, dv = 0 \tag{4.20}
\]

\[
\int_v [\mathbf{N}_1]^T \left( \frac{\partial \mathbf{\Phi}}{\partial \mathbf{\sigma}} \right) d\mathbf{\sigma} + \frac{\partial \mathbf{\Phi}}{\partial \mathbf{\sigma}_y} d\mathbf{\sigma}_y + \frac{\partial \mathbf{\Phi}}{\partial f} \, df \, dv = 0 \tag{4.21}
\]

\[
\int_v \mathbf{H}^T [(1 - f) \mathbf{\sigma}_y \mathbf{d}\varepsilon^p - \mathbf{d}\lambda (\mathbf{\sigma} \cdot \frac{\partial \mathbf{\Phi}}{\partial \mathbf{\sigma}})] \, dv = 0. \tag{4.22}
\]

### 4.3.2 Numerical integration of the constitutive equations

In a finite element method the solution is achieved incrementally with the integration of the governing equations. To solve the nonlinear governing equations we use implicit method [1, 9]. In the time interval \([t_n, t_{n+1}]\), the stress \( \mathbf{\sigma}_{n+1} \) is at first calculated as

\[
\mathbf{\sigma}_{n+1} = \Delta \mathbf{R}^T \cdot \mathbf{\sigma}_n \cdot \Delta \mathbf{R} + \mathbf{C}^e \cdot (\Delta \mathbf{\epsilon} - \Delta \mathbf{\epsilon}^p) = \mathbf{\sigma}_{n+1}^e - \mathbf{C}^e \cdot \Delta \mathbf{\epsilon}^p \tag{4.23}
\]

where \( \mathbf{\sigma}_n \) is the known stress state of the previous step, \( \Delta \mathbf{\epsilon} \) the known strain increment, \( \mathbf{C}^e \) the elasticity matrix, \( \Delta \mathbf{R} \) is the rotation tensor of the increment and \( \mathbf{\sigma}_{n+1}^e = \Delta \mathbf{R}^T \cdot \mathbf{\sigma}_n \cdot \Delta \mathbf{R} + \mathbf{C}^e \cdot \Delta \mathbf{\epsilon} \) is the elastic trial stress. The plastic strain increment at time \( t_{n+1} \) is given by

\[
\Delta \mathbf{\epsilon}^p = \Delta \lambda \left( \frac{\partial \mathbf{\Phi}}{\partial \mathbf{\sigma}} \right)_{t=t_{n+1}} = \Delta \lambda \left( - \frac{\partial \mathbf{\Phi}}{3 \partial p} \mathbf{I} + \frac{\partial \mathbf{\Phi}}{\partial q} \mathbf{n} \right)_{t=t_{n+1}}, \tag{4.24}
\]

where \( \mathbf{n}_{t=t_{n+1}} = \mathbf{n}_{n+1} = \mathbf{n}^e_{n+1} = 3 \mathbf{S}^e/(2q^e) \), \( \mathbf{S}^e \) is the deviatoric stress of \( \mathbf{\sigma}^e \). As defined in Eqn. (4.2), the elastic trial stress can be written as:

\[
\mathbf{\sigma}_{n+1}^e = -p^e \mathbf{I} + q^e \mathbf{n}^e. \tag{4.25}
\]

Furthermore, we introduce the notation

\[
\Delta \mathbf{\epsilon}_p = -\Delta \lambda \left( \frac{\partial \mathbf{\Phi}}{\partial p} \right)_{t=t_{n+1}} \tag{4.26}
\]

\[
\Delta \mathbf{\epsilon}_q = \Delta \lambda \left( \frac{\partial \mathbf{\Phi}}{\partial q} \right)_{t=t_{n+1}}, \tag{4.27}
\]
then the expression of the incremental plastic strain is given by

$$\Delta\varepsilon^p = \frac{1}{3}\Delta\varepsilon_p I + \Delta\varepsilon_q n_{n+1}^e. \quad (4.28)$$

Substituting equation (4.24) into equation (4.23), we find

$$\sigma_{n+1} = \sigma_{n+1}^e - K\Delta\varepsilon_p I - 2G\Delta\varepsilon_q n_{n+1}^e = -(p^e + K\Delta\varepsilon_p)I + (q^e - 3G\Delta\varepsilon_q)n_{n+1}^e, \quad (4.29)$$

where $K$, $G$ are the elastic bulk and shear moduli. Defining

$$p = p^e + K\Delta\varepsilon_p, \quad (4.30)$$
$$q = q^e - 3G\Delta\varepsilon_q, \quad (4.31)$$

the equation (4.29) can be rewritten as:

$$\sigma_{n+1} = -pI + qn_{n+1}^e. \quad (4.32)$$

Substituting the Eqns. (4.30,4.31) into Eqns. (4.26,4.27), we find

$$\Delta\varepsilon_q = \frac{2\Delta\lambda q^e}{\sigma_y^2 + 6G\Delta\lambda}, \quad (4.33)$$
$$\Delta\varepsilon_p = -\frac{3f\Delta\lambda}{\sigma_y} \sinh \left[ \frac{3(p^e + K\Delta\varepsilon_p)}{2\sigma_y} \right]. \quad (4.34)$$

Since in the time step $[t_n, t_{n+1}]$, $\Delta\lambda$, $\Delta\varepsilon_p$ and $q^e$ are known, then Eqn. (4.33) is solved. Eqn. (4.34) can be solved by using Newton iteration method. With known $\Delta\varepsilon_q$, $\Delta\varepsilon_p$ and $n_{n+1}^e$, $\sigma_{n+1}$ is determined by Eqn. (4.32). It is noted that all calculations are performed under the current configuration considering the finite strain assumptions.

### 4.3.3 Plastic loading/unloading conditions

In a continuum formulation, the Kuhn-Tucher conditions

$$\dot{\lambda} \geq 0; \quad \Phi(\varepsilon^p) \leq 0; \quad \dot{\lambda}\Phi(\varepsilon^p) = 0 \quad (4.35)$$

must be fulfilled at every point of the continuum. Since the yield condition is enforced globally, rather than locally, by integration of variational equation, some cares should be taken to the loading/unloading conditions.
The plastic multiplier vector $\mathbf{A}_{\text{internal}}$ denotes the value of $\lambda$ on the four Gauss points of each element. It is an internal vector in an element. At the integration points, if $\Phi < 0$, the Gauss point is elastic and $\lambda$ is forced to zero. It follows that the second and third governing equations become trivial. On the other case, if $\Phi > 0$, the point is judged plastic and the governing equation $\int_v \mathbf{N}^T T \Phi(\varepsilon^p, \nabla^2 \varepsilon^p) dv = 0$ is satisfied. When the three governing equations are solved, $\lambda$ is positive and great than zero. The condition $\lambda \Phi(\varepsilon^p) = 0$ is achieved at all plastic integration points.

In the 8-nodal $C^1$-continuous Hermite element, Vanishing of the global residual vector, $\int_v \mathbf{H}^T [(1 - f) \sigma_y \varepsilon^p - \sigma_{ij} \frac{\partial \Phi}{\partial \sigma_{ij}} \lambda] dv$, follows that the values $(1 - f) \sigma_y \varepsilon^p - \sigma_{ij} \frac{\partial \Phi}{\partial \sigma_{ij}} \lambda$, approaches zero at all plastic Gauss points in the element. Thus the classical Kuhn-Tucker conditions (4.35) are fulfilled. The integral formulation is equivalent to the deterministic condition. The discrete Kuhn-Tucker conditions suggested by Ramaswamy and Aravas [66] can be avoided.

4.3.4 Calculation of the tangent stiffness matrix

In the Newton iteration method one must provide the tangent matrix of the nonlinear algebraic equations to obtain the new incremental solution. In the finite element method the stiffness matrix must be renewed after each iteration when the full Newton method [1] is applied. From Equation (4.23) we get

$$d\mathbf{\sigma} = \frac{\partial \mathbf{\sigma}}{\partial \varepsilon} d\varepsilon + \frac{\partial \mathbf{\sigma}}{\partial \lambda} d\lambda + \frac{\partial \mathbf{\sigma}}{\partial \sigma_y} (h_p d\varepsilon^p - g d\nabla^2 \varepsilon^p)$$

(4.36)

Substituting the equation above into (4.20), (4.21) and (4.22) we rewrite the governing equations of the finite element method as

$$
\begin{bmatrix}
K_{uu} & K_{ul} & K_{ue} \\
K_{lu} & K_{ll} & K_{le} \\
K_{eu} & K_{el} & K_{ee}
\end{bmatrix}
\begin{bmatrix}
d\mathbf{u} \\
d\lambda \\
d\mathbf{\gamma}
\end{bmatrix} =
\begin{bmatrix}
\mathbf{R}_{\text{load}} \\
\mathbf{f}_\lambda \\
\mathbf{f}_\varepsilon
\end{bmatrix}
$$

(4.37)

where

$$K_{uu} = \int_v \left[ \mathbf{B}^T \left( \frac{\partial \mathbf{\sigma}}{\partial \varepsilon} \right) \mathbf{B} - \mathbf{\sigma} \cdot \left( 2 \mathbf{B}^T \mathbf{B} - \left( \frac{\partial \mathbf{N}}{\partial \mathbf{x}} \right)^T \frac{\partial \mathbf{N}}{\partial \mathbf{x}} \right) \right] dv$$
\[ \mathbf{K}_{uu} = \int_{\Omega} [\mathbf{B}^T \mathbf{m}_x] \mathbf{H} \, dv \\
\mathbf{K}_{ue} = \int_{\Omega} [\mathbf{B}^T \mathbf{m}_\sigma (h_y \mathbf{H} - g \mathbf{P})] \, dv \\
\mathbf{K}_{lu} = -\int_{\Omega} N_1^T (\frac{\partial \Phi}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial \varepsilon}) + \frac{\partial \Phi}{\partial f} \frac{1 - f}{1 + \Delta \varepsilon_p} \frac{\partial \Delta \varepsilon_p}{\partial \varepsilon} \mathbf{B} \, dv \\
\mathbf{K}_{\lambda u} = -\int_{\Omega} N_1^T (\frac{\partial \Phi}{\partial \sigma} \cdot \mathbf{m}_x + \frac{\partial \Phi}{\partial f} \frac{1 - f}{1 + \Delta \varepsilon_p} \frac{\partial \Delta \varepsilon_p}{\partial \lambda} \mathbf{N}_1 \, dv \\
\mathbf{K}_{\lambda e} = -\int_{\Omega} N_1^T (\frac{\partial \Phi}{\partial \sigma} \cdot \mathbf{m}_\sigma + \frac{\partial \Phi}{\partial f} \frac{1 - f}{1 + \Delta \varepsilon_p} \frac{\partial \Delta \varepsilon_p}{\partial \sigma} \mathbf{N}_1) (h_y \mathbf{H} - g \mathbf{P}) \, dv \\
\mathbf{K}_{\varepsilon u} = \int_{\Omega} \mathbf{H}^T \mathbf{T}_u \mathbf{B} \, dv \\
\mathbf{K}_{\varepsilon \lambda} = \int_{\Omega} T_\lambda \mathbf{H}^T \mathbf{N}_1 \, dv \\
\mathbf{K}_{\varepsilon e} = \int_{\Omega} [T_\varepsilon h_y + (1 - f) \sigma_y] \mathbf{H}^T \mathbf{H} - g T_\varepsilon \mathbf{H}^T \mathbf{P} \, dv \\
\mathbf{f}_\lambda = \int_{\Omega} N_1 \hat{\Phi} (\hat{\sigma}, \hat{\varepsilon}^p, \nabla^2 \hat{\varepsilon}^p) \, dv \\
\mathbf{f}_e = \int_{\Omega} \mathbf{H} [(1 - f) \sigma_y \Delta \varepsilon^p - \Delta \lambda (\sigma \cdot \frac{\partial \Phi}{\partial \sigma})] \, dv \\
\mathbf{R}_{\text{load}} = \int_{\Omega} \mathbf{B}^T \mathbf{\sigma} \, dv + \int_{\partial \Omega} \mathbf{N}^T \mathbf{t} \, dv \\

In equations above \( \mathbf{B} \) is the strain-displacement relation matrix. The detailed expressions of the derivatives are summarized. \( \int_{\Omega} \mathbf{\sigma} \cdot \left( 2 \mathbf{B}^T \mathbf{B} - \left( \frac{\partial \mathbf{N}}{\partial \varepsilon} \right)^\top \frac{\partial \mathbf{N}}{\partial \varepsilon} \right) \, dv \) in \( \mathbf{K}_{uu} \) is the part of geometric stiffness matrix [1].

**Expressions in stiffness matrix and residual vector**

\[
\frac{\partial \sigma}{\partial \varepsilon} = \mathbf{D}^e - \mathbf{K}^e \frac{\partial \Delta \varepsilon_p}{\partial \varepsilon} - 2 \mathbf{G} \mathbf{n}^e \frac{\partial \Delta \varepsilon_q}{\partial \varepsilon} - 2 \mathbf{G} \Delta \varepsilon_q \frac{\partial \mathbf{n}^e}{\partial \varepsilon}
\]

\[
\mathbf{m}_\lambda = -\mathbf{K}^e \frac{\partial \Delta \varepsilon_p}{\partial \lambda} - 2 \mathbf{G} \frac{\partial \Delta \varepsilon_q}{\partial \sigma} \mathbf{n}^e
\]

\[
\mathbf{m}_\sigma = -\mathbf{K}^e \frac{\partial \Delta \varepsilon_p}{\partial \sigma} - 2 \mathbf{G} \frac{\partial \Delta \varepsilon_q}{\partial \sigma} \mathbf{n}^e
\]

\[
\mathbf{T}_u = [-\frac{B_u}{3} \mathbf{I} \frac{\partial \sigma}{\partial \varepsilon} + B_f \mathbf{A}_u + \frac{4q}{\sigma_y^2} \mathbf{n}^e \mathbf{m}_x] \Delta \lambda - \sigma_y \Delta \varepsilon^p \mathbf{A}_u
\]

\[
\mathbf{T}_\lambda = -[-\frac{B_u}{3} \mathbf{I} \mathbf{m}_x + B_f \mathbf{A}_\lambda + \frac{4q}{\sigma_y^2} \mathbf{n}^e \mathbf{m}_x] \Delta \lambda - (p \frac{\partial \Phi}{\partial p} + q \frac{\partial \Phi}{\partial q}) - \sigma_y \Delta \varepsilon^p \mathbf{A}_\lambda
\]

\[
\mathbf{T}_e = (1 - f) \Delta \varepsilon^p - \sigma_y \Delta \varepsilon^p \mathbf{A}_\sigma - \Delta \lambda [-\frac{B_u}{3} \mathbf{I} \mathbf{m}_\sigma + B_{\sigma} + B_f \mathbf{A}_\sigma + \frac{4q}{\sigma_y^2} \mathbf{n}^e \mathbf{m}_\sigma - \frac{4q^2}{\sigma_y^3}]
\]

\[
\mathbf{A}_u = \frac{1 - f}{1 + \Delta \varepsilon_p} \frac{\partial \Delta \varepsilon_p}{\partial \varepsilon}
\]
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\[ A_\lambda = \frac{1 - f}{1 + \Delta \varepsilon_p} \frac{\partial \Delta \varepsilon_p}{\partial \lambda} \]
\[ A_{\sigma_y} = \frac{1 - f}{1 + \Delta \varepsilon_p} \frac{\partial \Delta \varepsilon_p}{\partial \sigma_y} \]
\[ B_u = \frac{3f_1q_2}{\sigma_y} \sinh \left( \frac{3q_2 \sigma}{2\sigma_y} \right) + \frac{9pf_1q_2^2}{2\sigma_y^2} \cosh \left( \frac{3q_2 \sigma}{2\sigma_y} \right) \]
\[ B_{\sigma_y} = -\frac{3pf_1q_2}{\sigma_y^2} \sinh \left( \frac{3q_2 \sigma}{2\sigma_y} \right) - \frac{9p^2f_1q_2^2}{2\sigma_y^4} \cosh \left( \frac{3q_2 \sigma}{2\sigma_y} \right) \]
\[ B_f = \frac{3q_1q_2}{\sigma_y} \sinh \left( \frac{3q_2 \sigma}{2\sigma_y} \right) \]

The set of Eqn. (4.36) governs the element behaviour during plastic flow. If all elements are elastic, as suggested by Pamin [58], the vectors \( n \), \( f_\lambda \) as well as \( f_\varepsilon \) are set to zero. Therefore the submatrice, \( K_u \), \( K_{\lambda u} \), \( K_{\varepsilon u} \), \( K_{\lambda \varepsilon} \) and \( K_{\varepsilon \varepsilon} \) are equal to zero. \( K_{\lambda \lambda} \) and \( K_{\varepsilon \varepsilon} \) are determined by

\[ K_{\lambda \lambda} = \sum_{ip=1}^{4} E N_{1ip} N_{1ip}^T V_{ip} \quad (4.38) \]
\[ K_{\varepsilon \varepsilon} = \sum_{ip=1}^{4} E H_{ip} H_{ip}^T V_{ip} \quad (4.39) \]

4.3.5 Boundary conditions

Compared to the formulation of Von-Mises gradient plasticity, more nodal values are involved in the formulation of GTN damage gradient plasticity. Introducing additional gradients into governing equations, one needs set more boundary conditions to maintain uniqueness of the finite element equation. Note \( \Lambda \) is an internal vector in elements. The submatrix \( K_{\lambda \lambda} \) is a four rank matrix and has no zero eigenvalue. No boundary condition of \( \lambda \) need be involved in the formulation. Only the boundary condition of \( \varepsilon \) has been introduced. It is the same as the von-Mises gradient plasticity formulation.

It is state here again that Mühlhaus and Aifantis suggested to introduce

\[ \frac{\partial \varepsilon}{\partial n} = 0 \]

as additional boundary condition for all plastic boundary. For \( C^1 \) element, this condition
4.4. Mesh sensitivity analysis

4.4.1 Shear band analysis in combining with damage

Strain localization is observed only when the material possesses strain softening, which can be introduced either by the unstable stress-strain relation or caused by, for instance, void growth. In this section, shear band evolution in ductile damage process is investigated using the nonlocal GTN model.

We consider a rectangular unit cell with an initial length $A_0$ and width $B_0$. Plane strain loading conditions are assumed here. The unit cell represents a material with a doubly periodic array of soft spots, containing initial porosity, as has also been studied by Tvergaard and Needleman [86]. The soft spot locates at the bottom left corner of the cell and the area of the soft spot is $(0.1A_0) \times (0.1B_0)$. Symmetric boundary conditions are applied on all edges,

\begin{align}
    u_x &= 0 \quad \text{at } x = 0 \quad (4.40) \\
    u_y &= 0 \quad \text{at } y = 0 \quad (4.41)
\end{align}
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Figure 4.1: Mesh distortions in shear band analysis with the nonlocal GTN model. Three different finite element meshes with 10 x 10, 20 x 20 and 40 x 40 elements are used. (a) Without strain gradient regulator; (b) with strain gradient regulator $l = 0.02B_0$, where $B_0$ stands for the initial specimen height.

\begin{align*}
  u_y &= U_1 \quad \text{at} \quad y = B_0 \\
  u_x &= U_2 \quad \text{at} \quad x = A_0
\end{align*}

(4.42) (4.43)

where $u_x$, $u_y$ are the displacement components in the $x$ and $y$ direction, respectively. $U_1$, $U_2$ are the given displacements. In this analysis, only $U_1$ is prescribed. $U_2$ is not given but keeps the form of the boundary. The initial porosity distribution in the soft spot is specified to 0.05 and strain controlled nucleation is assumed in the whole domain except the soft spot with $f_N = 0.04$, $\varepsilon_N = 0.3$, $S_N = 0.1$ in equation (4.14). Young's modulus is $E = 300\sigma_0$, Poisson's ratio $\mu = 0.3$, $q_1$, $q$ in Eqn (4.1) are assumed to be $q_1 = 1.5$, $q_2 = 1$. Finite strains are taken into account. The stress-plastic strain relation is assumed as a power law,

\[ \frac{\bar{\sigma}}{\sigma_0} = \left( \frac{3G}{\sigma_0 e^p} \right)^N \]  

(4.44)
Mesh sensitivity analysis

Figure 4.2: Overall stress-strain curves in shear band analysis with the nonlocal GTN model. Three different FE meshes are used with \( l = 0 \) and \( l = 0.02B_0 \), respectively.

where \( N = 0.1 \), \( G \) is shear modulus. The yield stress is determined by

\[
\sigma_y = \bar{\sigma} - g \nabla^2 \bar{\varepsilon}^p = \sigma_0 \left[ \left( \frac{3G}{\sigma_0} \bar{\varepsilon}^p \right)^N - l^2 \nabla^2 \bar{\varepsilon}^p \right].
\] (4.45)

Figure 4.2 shows the overall stress-strain curves with the classical GTN model as well as the modified GTN model coupled to the gradient plasticity with \( l = 0.02B_0 \), respectively. Results are shown for \( A_0/B_0 = 1.5 \) using three uniform meshes consisting of from \( 10 \times 10 \), \( 20 \times 20 \), \( 40 \times 40 \) quadrilateral 8-nodal elements. It is clear that the post-localization response is very sensitive to the mesh resolution without the gradient regulator. The finer are the elements, the lower the stress levels will be (Fig. 4.2). Under gradient plasticity all three different meshes show a numerically unique solution, as we learned from the results of the strain softening analysis.

Mesh distortions with and without strain gradient regulator are shown in Fig. 4.1. Without the gradient regulator \( (l = 0) \), the shear band develops within a layer of elements, that is, the shear band width is as narrow as an element size. For a finer mesh, one needs less energy and so less applied load to reach the given local plastic strain state, which is related to the material porosity. By introducing the gradient term into the constitutive equation, the local strain state is affected by its local variations. Fig. 4.1(b) shows the mesh distortions...
Nonlocal GTN damage model based on gradient plasticity

Figure 4.3: Variations of the porosity and plastic strain from shear band analysis using the GTN model with \( l = 0.02B_0 \). The overall mean strain \( \epsilon_{yy} = \Delta B/B_0 = 0.25 \) (a) Void volume distribution versus \( x \) at \( y = 0.4B_0 \); (b) Effective plastic strain distribution versus \( x \) at \( y = 0.4B_0 \).

with \( l = 0.02B_0 \) are independent of element sizes. Shear band is uniquely described by the material parameter \( l \) and the applied loading condition, instead of the finite element size.

Figures 4.3 and 4.4 display distributions of the void volume fraction \( f \) and the equivalent plastic strain cross the shear band, with \( l = 0.02B_0 \) and \( l = 0.04B_0 \), respectively. Using the classical GTN model, the variations of the void volume fraction and the equivalent plastic strain are restricted in a band as narrow as an element size. Within the frame of gradient plasticity the curves are characterized by the parameter \( l \). With the increasing material length parameter \( l \), the region of the high porosity and high plastic strain grow.

The strength of the specimen increases with \( l \), as plotted in Fig. 4.5. By smoothing the plastic strain distribution, the material becomes stronger, which slows down development of voids and so the damage zone.
Figure 4.4: Variations of the porosity and plastic strain from shear band analysis using the GTN model with $l = 0.04B_0$. The overall mean strain $\epsilon_{yy} = \Delta B/B_0 = 0.25$ (a) Void volume distribution versus $x$ at $y = 0.4B_0$; (b) Effective plastic strain distribution versus $x$ at $y = 0.4B_0$.

Figure 4.5: Effects of the intrinsic material length scale parameter $l$ from the shear band analysis using the GTN model.
4.4.2 Failure analysis of bars with a central hole

We consider a rectangular specimen with a central hole which has been analyzed in Chap. 3. Now the nonlocal GTN model is applied. Due to symmetry only one fourth of the specimen is discretised as shown in Fig. 4.6. The specimen is subjected to tensile loading along the Y direction under plane strain conditions. The initial porosity is \( f_0 = 0.05 \) and the void nucleation is not considered. The same values of Young’s modulus \( E \), Poisson’s ratio \( \mu \) and the stress-strain relation as in the shear band analysis are used. To analyze the mesh sensitivity of the specimen’s failure, the effects of rapid void coalescence is taken into account.

The void volume function \( f \) is replace by \( f^* \), which is defined as

\[
  f^* = \begin{cases} 
  f & \text{if } f \leq f_c; \\
  f_c + \frac{f - f_c}{f_f - f_c} (f - f_c) & \text{if } f \geq f_c. 
  \end{cases} 
\]  

The onset of rapid void coalescence is assumed to begin at a critical void volume fraction, \( f_c \), with \( f_{\text{in}}^* \) being the value of \( f^* \) at zero stress, i.e. \( f_{\text{in}}^* = 1/q_1 \). As \( f \to f_f \), \( f^* \to f_{\text{in}}^* \) and the material loses all loading capacity. The parameters are given by \( q_1 = 1.5, q_2 = 1, f_f = 0.388, f_c = 0.15 \). To prevent numerical difficulties occurring at failure, we
assume that the flow stress is ten percent of the initial yield stress at failure. It means the material cannot lose all loading capacity at failure.

Using different material length parameter \( l \) does not change the failure mechanism of the material but delay the material failure and remove the mesh-dependence. Figure 4.7 shows that the failure begins at the bottom of the mesh near the hole and extends outside along the bottom of the mesh. Whereas the maximum porosity develops towards the maximum shear direction, the final material failure occurs at the symmetric plane. The intrinsic material length does not change the global distribution of the porosity.

The overall stress-strain diagrams with and without regulation of plastic strain gradient using three different finite element meshes are plotted in Fig. 4.8. For the classical GTN model with \( l = 0 \) the critical loading point for void growth is effected by the mesh size. For the finer mesh the specimen reaches the critical point earlier than the coarser mesh does. The deviation is proportional to strain gradients. One may expect much stronger mesh-dependence in crack analysis. The mesh sensitivity is removed by adding the gradient regulator if the element size is smaller than that the material length needs. As shown in Fig. 4.8, for \( l = 0.04B \) the mean stress-mean strain curves with 500 and 825 elements are unique. The coarse mesh shows slight mesh-dependence due to too coarse elements.

Fig. 4.9 shows the influence of the gradient parameter on the stress-strain curve using the 500 elements mesh. With the increasing value of the material length parameter, the
Figure 4.8: Overall stress-strain curves with three finite element meshes for the center holed specimen using the nonlocal GTN model, with $l = 0$ and $l = 0.04B_0$, respectively.

Figure 4.9: Effects of the intrinsic material length scale parameter $l$ on failure analysis of the center holed specimen using the nonlocal GTN model.
4.5. Microscopic strain fields in multiphase metallic alloys

Material strength increases significantly and the material failure is delayed. The influence of gradient plasticity in Figure 4.9 represents some kinds of size effects in material failure, as observed in experiments [34]. For a given material, that is, for a given intrinsic material length, the material strength varies with the specimen geometry: the smaller specimens have higher strength than the larger ones.

The present GTN model based on the gradient plasticity provides a tendentious prediction about size effects in material failure. To obtain a quantitative agreement, much detailed computations and experimental efforts are needed. Furthermore, the finite element mesh must be finer than the certain size determined by the intrinsic material length \( l \).

In this chapter, computational analysis of ductile material failure shows that a mesh-independent solution can be achieved by incorporating the strain gradients into the micromechanical constitutive equations. The fact that increase of the material strength will delay the computational material failure prediction is consistent to the known size effects in ductile materials. The gradient plasticity has the potential to give a more reliable and more accurate prediction of material failure.

4.5 Microscopic strain fields in multiphase metallic alloys

Three parameters are introduced in the GTN yield function by Tvergaard and Needleman [82, 83, 85] to take care of interactions of voids and improve its predictions. Nevertheless, An essential question is the transferability of the three parameters of the model under varying conditions of stress triaxiality. In order to study the effect finite element computations of a cell model, i.e. a unit cylinder containing a spherical hole have been performed by many researchers [17, 84, 74, 41, 96, 55, 90]. The numerical 'mesoscopic' stress, strain, and void growth responses are then compared with the predictions of the GTN model. The parameters are chosen in the way that the responses of the homogeneous constitutive model fit the responses of the cell model best.
In this section, it is not investigated whether the three parameters are material parameters or not and how to quantify the parameters under different loading conditions. The aim here is that the cell model analyzed by other researchers is applied to consider the effect of gradient plasticity. The influence of gradient plasticity on the 'mesoscopic' strain fields is performed and analyzed.

### 4.5.1 Cell model

The mechanical behaviour of porous solids can be simulated by cell model calculations. Koplik et al. [41] and Brocks et al. [17] adopted an axisymmetrical cylindrical unit cell with one void in it to study void growth under different given stress triaxialities, in order to examine GTN damage model, and, to fit the three parameters of the modified GTN damage model.

The continuum considered here consists of a periodic assemblage of hexagonal cylindrical unit cells which are approximated by spherical cylinders. The porous solid is plotted in Fig. 4.10. Furthermore, the hexagonal cylinder is simplified as axisymmetrical cylindrical unit cell with a spherical void in it. Every cell has the initial length $2L_0$ and radius $R_0$ and
the radius of the spherical hole is \( r_0 \). The cell is subjected to homogeneous radial and axial displacements, \( u_1 \) and \( u_3 \).

The 'mesoscopic' principle strains and the effective strain are given by:

\[
E_1 = E_2 = \ln\left( \frac{R}{R_0} \right); \quad E_3 = \ln\left( \frac{L}{L_0} \right); \quad E_e = \frac{2}{3} |E_3 - E_1|. \tag{4.47}
\]

The corresponding 'mesoscopic' true principal stresses, \( \Sigma_1, \Sigma_2, \Sigma_3 \), are the average reaction forces at the cell boundaries per momentary areas. Effective stress, hydrostatic stress and triaxiality result in:

\[
\Sigma_e = |\Sigma_3 - \Sigma_1|; \quad \Sigma_h = \frac{1}{3}(\Sigma_3 + 2\Sigma_1); \quad T = \frac{\Sigma_h}{\Sigma_e} \tag{4.48}
\]

For elastic-plastic matrix material there is just one structural void in the center of the cell, hence the initial void volume fraction, \( f_0 \), is given as:

\[
f_0 = \frac{2r_0^3}{3R_0^2L_0}. \tag{4.49}
\]

The current cell volume is:

\[
V = 2\pi R^2 L. \tag{4.50}
\]

The current void volume fraction \( f \) can be expressed using the condition of incompressibility for plastic deformation:

\[
(1 - f)V - \Delta V^e = (1 - f_0)V_0 \tag{4.51}
\]

where \( \Delta V^e \) is the volume increase of the cylindrical cell due to the elastic dilatation arising from the imposed hydrostatic stress which is approximated by Koplik, Needleman [41] and Brocks et al. [17]:

\[
\Delta V^e = V_0(1 - f_0)\frac{3(1 - 2\mu)}{E}\Sigma_h. \tag{4.52}
\]

Here \( E \) and \( \mu \) are Young's modulus and Poison ratio, respectively.

To keep triaxiality constant during the loading history, the ratio of \( \Sigma_3/\Sigma_1 \) should remain constant, whereas the ratio of the prescribed strains, \( E_3/E_1 \), will vary with time. If \( T \) is constant, then \( \Sigma_1 \) and \( \Sigma_3 \) has the following relation:

\[
\Sigma_1 = \left( \frac{3T - 1}{3T + 2} \right) \Sigma_3. \tag{4.53}
\]
The cell is discretized by a 400-elements mesh in Fig. 4.11. Axisymmetric condition is enforced. The structure is subjected to a homogeneous elongation $u_3$ in axial direction. The radial displacement is kept homogeneous too, by constraint condition. A special user supplied load routine has been written for the FE program ABAQUS to guarantee a constant $\Sigma_3/\Sigma_1$ ratio. This is realized by the user subroutine interface MPC which defines multi-point constraints supported by ABAQUS. In this subroutine two spring elements in axial and radial directions are introduced to measure the axial stress $\Sigma_3$ and radial stress $\Sigma_1$. In our computations the cell model which has been performed by Koplik et al [41] is investigated by means of introducing the Laplacian of effective plastic strain $\nabla^2 \varepsilon^p$ into flow stress, while the first-order gradient of plastic strain, $|\nabla \varepsilon^p|$ is omitted.

Figure 4.11: Finite element mesh of a cell. Due to symmetry only 1/4 part of the cylindrical unit cell with a spherical void is discretized. The two springs in the mesh is used to keep the constant triaxiality during loading by means of a user element subroutine MPC in ABAQUS. $f_0 = 0.0013$

4.5.2 Influence of gradient plasticity on the strain fields

In this part we investigate the parameter dependence of void growth in proportional stressing history using the axisymmetric cell model. The varied parameters are stress state triaxiality,
matrix material strain hardening and intrinsic length of material. The stress-strain relation is given as power-law hardening:

$$\bar{\sigma} = \sigma_0 \left( \frac{E e^p}{\sigma_0} \right)^N$$

(4.54)

where $N$ is the strain exponent and assumed to be $N = 1/10$. $\sigma_0$ is the initial yield stress and Young's modulus $E$ is $E = 500\sigma_0$. Poisson ratio $\nu$ is $1/3$. In this analysis the initial void volume fraction is set to $0.0013 (f = 0.0013)$. It represents the case of high density porous ductile material. The stress triaxiality is changed from 1 to 3. Different intrinsic length scales, $l = 0, l = 0.358r_0, l = 0.566r_0$ and $l = 0.8r_0$ are used to analyze the effects of plastic strain gradients on the deformation field.

![Graph](image)

Figure 4.12: The 'mesoscopic' effective stress vs effective strain for varying stress triaxiality and different intrinsic length scales. a): nominal effective stress vs effective strain. b): nominal effective stress vs nominal effective strain, $E_e^0$ is the effective strain at the onset of cell collapse without material length scale ($l=0$)

Triaxiality ratios $1 \leq T \leq 3$ are applied covering the range from rather blunt notched bar specimens ($T \approx 1$) to the triaxiality prevailing in crack tip fields for lightly hardening solids ($T \approx 3$) [41]. Fig. 4.12 shows various influences of different material lengths in macro-stress variation with macro-strain $E$ when the stress triaxiality $T$ is set to 1, 2, 3, respectively. It is expected that the pre-necking curves are not changed by the effects of gradient terms due to small deformation gradient under different loading conditions. The strength of material
increases significantly in post-necking with the strong effect of the plastic strain gradients. For the three loading conditions \((T = 1, 2, 3)\), when \(l\) is in the magnitude of the radius of voids, \(r_0\), the size effect of material strength is strong and material collapse is delayed noticeably. This prediction coincides with [92] although different boundary conditions are set.

Fig. 4.13a shows the 'mesoscopic' effective stress vs effective strain curve for \(T = 1\). The damage evolution vs 'mesoscopic' effective strain is plotted in Fig. 4.13b. With the increase of material length, the void growth decreases. It means that the strength of material increases and the failure of material caused by void growth delays due to slow growth of void volume fraction. Fig. 4.13c illustrates the reduction of area vs mesoscopic effective strain curves for \(T = 1\) using different intrinsic length \(l\). The last figure shows that an effective strain is eventually reached at which the cell radius remains constant. It implies that further deformations take place in a uniaxial straining mode which corresponds to flow localization into the ligament between radially adjacent voids. The involvement of material length in the flow stress does not qualitatively change the cell collapse, but postpone the collapse point significantly later with the increase of material length value.

Fig. 4.14 and 4.15 summarize computational results for the stress triaxiality \(T = 2\) and \(T = 3\), respectively. It can be concluded from these figures that the introduction of plastic strain gradient in yield function influences the strain fields of the cell and makes it more 'diffused' and 'homogeneous'. Effects of plastic strain gradients arise the material strength, slow down the damage evolution and delay the collapse of the cell. The gradient plasticity theory can affect the micro-scale deformation field of material and then predict the size effect of material behaviour in macro-scale level when the material length is determined from the micromechanical analysis.

From these figures the range of material length can be determined. When the material length \(l\) is almost equals to \(1/3r_0\), the size effect of material strength is obvious. For \(l = 0.8r_0\), the size effects of material strength depends on specimen size significantly for different stress triaxiality. In this case it means that the material length less than the radius of voids can predict the size effects of material failure for the high density porous ductile material.
Figure 4.13: Finite element results for $L_0/R_0 = 1.0$, $f_0 = 0.0013$ with stress triaxiality $T = 1.0$. a) Mesoscopic effective stress vs effective strain response. b) Void volume fraction vs effective strain. c) Reduce of area vs effective plastic strain. Different length scales are used.
Figure 4.14: Finite element results for $L_0/R_0 = 1.0$, $f_0 = 0.0013$ with stress triaxiality $T = 2.0$. a) 'Mesoscopic' effective stress vs effective strain response. b) Void volume fraction vs effective strain. c) Reduce of area vs effective plastic strain. Different length scales are used.
Figure 4.15: Finite element results for $L_0/R_0 = 1.0$, $f_0 = 0.0013$ with stress triaxiality $T = 3.0$. a) 'Mesoscopic' effective stress vs effective strain response. b) Void volume fraction vs effective strain. c) Reduce of area vs effective plastic strain. Different length scales are used.
Nonlocal GTN damage model based on gradient plasticity
Chapter 5

Application of computational gradient plasticity: Simulation of micro-indentation based on gradient plasticity

Recently, experiments on micro- and nano-indentation hardness tests have been extensively adopted for determining material characteristics in micro-dimension [49, 50, 65, 70]. It has been found that the micro-hardness of materials is significantly higher than the macro-hardness by a factor of two or more in the range from about 10 microns to 0.1 micron. Generally, it can be said the smaller the scale, the stronger will be the solid. Based on experimental observations Nix and Gao [56] predict a linear dependence of the square of the micro-hardness, $H$, and the inverse of the indentation depth, $1/h$, that is,

$$\left(\frac{H}{H_0}\right)^2 = 1 + \frac{h^*}{h}, \quad (5.1)$$

where $H_0$ is the macro-hardness and $h^*$ is a material specific parameter depending on indenter angle as well as on the mechanical property of materials. Nix and Gao [56] suggest $h^* = 3(\cos \beta)^2/(16\rho_s)$, where $b$ is the Burgers vector and $\rho_s$ is the statistically stored dislocation density. The statistically stored dislocations are related to the plastic strain.
Consequently the micro-hardness is related to the indentation depth through the statistically stored dislocations $\rho_s$. It is verified that Equation (5.1) can be used to predict the size effect of micro-hardness for many kinds of metallic materials [32, 37, 56].

In conventional continuum mechanics the whole stress and displacement fields are independent of the absolute geometry size. Should the indenter be sharp enough and should the specimen be large enough, the stress filed near the indenter tip can be scaled by the indentation depth. That is, the hardness computed in conventional continuum mechanics is a constant due to the geometrical similarity. Hence the strain gradient effect should be considered into nano- and micro-indentation simulations. According to the authors' knowledge, no result of the depth-dependent micro-indentation using high order gradients of plastic strains (Aifantis gradient plasticity theory) has been reported. The aim of this chapter is to investigate effects of the strain gradients in micro-indentation simulations and to check whether or not the phenomenological gradient plasticity model can capture the depth-dependence of the micro-hardness. Furthermore, we are going to examine the relationship between the micro-hardness and the indentation depth as proposed by Eqn. (5.1). In this sense the parameter $h^*$ is used as a fitting parameter in the gradient plasticity model based on suitable assumptions. The role of the first-order and the second-order derivatives of equivalent plastic strain is systematically investigated.

## 5.1 Modeling

It is assumed that the uniaxial stress-strain relation can be described by a power-law hardening as

$$\tilde{\sigma} = \sigma_0 \left( \frac{E\tilde{\varepsilon}^p}{\sigma_0} \right)^N,$$

where $E$ is Young's modulus, $N \leq 1$ is the plastic strain hardening exponent, $\sigma_0$ is the initial yield stress and $\tilde{\varepsilon}^p$ is the equivalent plastic strain.

To simplify computational modeling the indenter is assumed to be axisymmetric conical. The half angle of the axisymmetric indenter is taken to be $72^\circ$, which correspond to Berkovich indenter (Fig. 5.1). This assumption has been adopted by many previous micro-
indentation simulations based on other different gradient plasticity models [14, 56, 93]. 3D effects to such simplification have been discussed in [45]. The contact radius is defined as \( a \) and the depth of penetration of the indenter is \( \delta \). The indenter is assumed to be rigid. The contact between the indenter and the work piece is postulated frictionless.

![Axisymmetric micro-indentation model](image)

Figure 5.1: Axisymmetric micro-indentation model used in the present computations. \( \beta \) denotes the half angle of indenter, \( h \) is the indentation depth and \( \delta \) the displacement of indenter, \( a \) the radius of the contact area of the indentation, \( a_0 \) a global measurement of the specimen.

To make use of the contact element technique in ABAQUS and to visualize the finite element results, an additional sheet of conventional isoparametric elements is embed on the user element mesh with vanishingly small strength. It makes also possible to evaluate the reaction forces and strain distributions in the specimen.

The contact radius of indentation, \( a \), can be determined by the vanishing contact force computed by ABAQUS. Due to the scattering of the \( a \) value proportional to the element size near the indenter tip, the final radius value must be smoothed. As soon as \( a \) is known, the indentation depth is calculated as

\[ h = \frac{a}{\tan \beta}. \]  

\[ (5.3) \]
Using the force applied on the indenter, $P$, the hardness is computed as

$$H = \frac{P}{\pi a^2}. \quad (5.4)$$

This method can be taken for all possible indenter angles and different indentation depths.

The remote radius $a_0$ is introduced to get non-dimensional computation. $a_0$ should be large enough in comparing with $a$. To obtain the macro hardness value, if the mesh used for computations is fine enough, the final results of macro-hardness are independent of $a_0$.

In this chapter different finite element meshes are used to study the mesh-(in)dependence. It is confirmed that computational results under finite strain assumption are numerically mesh-insensitive when the contact surface is discretised by more than 10 elements. The scattering due to discrete element size is limited in 5% for performed computations. In this chapter we just report numerical results with a kernel mesh of $30 \times 20$ 8-nodal gradient plasticity elements near to the indenter tip. It means that only in this kernel mesh the gradient plasticity theory is applied. The conventional 8-nodal displacement element is used in the outer mesh due to the small plastic strain and its gradients. The mesh is show in Fig. 5.2. In computations the absolute element size near the indenter tip varies with the given intrinsic material length scale proportionally. The final computational step just reaches half of the kernel. The whole mesh has a size as large as ten times of the kernel and the overall mesh size is defined as $a_0$ in our computations.

In most computational work on gradient plasticity published by de Borst and co-workers [24, 58], only the Laplacian of equivalent plastic strain was introduced into the constitutive relationship and flow stress, namely

$$\sigma_y = \tilde{\sigma}(\tilde{\varepsilon}) - g \nabla^2 \tilde{\varepsilon} \quad \text{with} \quad g = \sigma_0 l f(\tilde{\varepsilon}).$$

In the analysis of strain-softening, Pamin [58] suggested the gradient parameter $f = -\tilde{\sigma}'(\tilde{\varepsilon})$, where $-\tilde{\sigma}'(\tilde{\varepsilon})$ is the slope of the stress-strain curve measured in uniaxial tests. Such assumption leads to a smooth increasing and decreasing of the gradients of plastic strain in computations. It is specially of importance as soon as the strains are concentrated increasingly. Ramaswamy [66], Sverberg [78] and Mikkelsen [52] use $f = 1$ in the shear band analysis for strain-hardening material. As stated by Pamin [58], in the shear band, where intensive shearing occurs, $\nabla^2 \tilde{\varepsilon}$ is negative, thus the gradient term will arise the flow stress there, while $\nabla^2 \tilde{\varepsilon}$ becomes positive near the elastic-plastic boundary, which makes it possi-
Figure 5.2: A typical finite element mesh with $C^1$ continuity, with 650 elements and 3700 nodes, used for computations. All elements have 8 nodes for interpolation of displacement and 4 additional nodes for the effective plastic strain. The indenter is simulated with a rigid surface. (a) full mesh. (b) elements near to the indenter tip.

ble for the localization zone to spread out the plastic zone due to the decrease of the flow stress. Furthermore, from torsion solutions one may conduct that the parameter $g$ must be a function of the plastic strain to avoid singular strain distribution.

In the numerical analysis of micro-indentation, it is observed that in the area near the indenter tip, the Laplacian of the equivalent plastic strain oscillates strongly and $l^2 \nabla^2 \varepsilon^p$ is over hundreds times of the strain itself. Similar phenomena can be found in crack tip field analysis of ductile material. It implies that using a constant parameter $g$ makes numerical computations difficult.

Generally we assume that, when the equivalent plastic strain is small, the influence of $\nabla^2 \varepsilon^p$ should not be very strong on the strength of material in the area near the indenter tip. For large plastic strains the amplitude of $g$ should be limited and positive, i.e.,

$$f_2(\varepsilon^p) = \begin{cases} 
\left( \frac{\varepsilon^p}{\varepsilon_0^p} \right)^n & \text{if } \varepsilon^p \leq \varepsilon_0^p \\
1 & \text{if } \varepsilon^p > \varepsilon_0^p \end{cases}$$

(5.5)

Above two parameters, the exponent $n$ and the range $\varepsilon_0^p$ are introduced. Computations with $1 < n < 3$ show a stable numerical convergence. The final computational results are slightly
affected by \( n \) and \( \varepsilon_0^p \) values. In computations reported in this chapter we set \( n = 2 \) and \( \varepsilon_0^p = 0.1 \). This assumption will not change our conclusions.

5.2 Results

The initial input data adopted in the present computations are taken from the paper of Bergley and Hutchinson [14], with plastic strain hardening exponents \( N = 1/3 \), \( N = 1/5 \) and \( N = 1/10 \), Young’s modulus \( E = 300\sigma_0 \) and Poisson’s ratio \( \nu = 0.3 \). For these parameters the finite element computations predict macro-hardness of \( H_0 = 7.89\sigma_0 \), \( 5.28\sigma_0 \) and \( 3.89\sigma_0 \) for \( N = 1/3 \), \( 1/5 \) and \( 1/10 \), respectively, under finite strain assumptions and plastic flow theory. These predictions agree with the results of Begley and Hutchinson [14].

It is worth noting that to avoid artificial effects in numerical fitting, we did not take any additional fitting algorithm in hardness evaluation. The scattering of the data is caused by finite element discretization. The contact area is directly evaluated from the contact elements and, therefore, spreads discontinuously. This scattering grows with the strain exponent \( N \). For materials with higher plastic strain hardening, the scattering is larger.

5.2.1 Role of the Laplacian of the plastic strain

In this subsection we assume \( l_1 = 0 \) and study effects of the second-order derivative (Laplacian) of equivalent plastic strain, \( \ell \), only. The assumption in (5.5) is introduced. The micro-hardness \( H \) over macro-hardness \( H_0 \) is plotted as a function of indentation depth \( h \) in Fig. 5.3. In the figures the symbols denote the computational results and the solid lines are fitting according to suggestion of Nix and Gao [56]. Variations about \( \ell \) are shown for \( N = 1/10 \) in Fig. 5.3(a). The gradient regulator \( \ell \) arises the strength of the continuum model and so the hardness. For the same macro-hardness, the micro-hardness for small \( h \) from the finite element computations is significantly larger than Nix and Gao’s prediction.

In Fig. 5.3(b) the depth is normalized by the intrinsic material length \( l \). These figures verifies that the micro-hardness explicitly depends on \( h/l \), i.e. \( H = H_0\psi(h/l) \). Influence of
Results

Figure 5.3: Depth-dependence of the micro-hardness. The symbols stand for computational finite element results. Lines are predictions of Nix and Gao [56]. Only the Laplacian of plastic strain is considered into the formulation of the flow stress ($l_1 = 0$). (a) Effects of intrinsic material length $l$. (b) Effects of strain hardening exponent $N$.

the parameter $l$ can be scaled if the horizontal axis is normalized by $l$.

From Nix and Gao [56] it is known that $H^2$ is a linear function of $1/h$. In Fig. 5.4 the normalized hardness is plotted as function of $l/h$. Figure 5.4(a) depicts that the correlation between $H^2$ and $1/h$ is nonlinear. The solid lines are a least square fitting of the computational results. The Aifantis’ model with Laplacian gradient regulator provides a significant overestimate in comparison with experimental fitting for some metals in [56].

It is interesting to note in Fig. 5.4(b) that the present results are similar to those obtained using Fleck-Hutchinson strain gradient plasticity model in [14]. According to Beglecy and Hutchinson [14] the computational prediction of micro-hardness is approximated by a linear function, that is,

$$\frac{H}{H_0} = 1 + c^* \left( n, \frac{\sigma_0}{E} \right) \frac{l}{h},$$

where $c^* (n, \sigma_0 / E)$ is a coefficient depending on mechanical property of materials. For the present computations the linear fitting is valid only for $l/h \geq 1$. 
5.2.2 Role of the first-order derivative of the plastic strain

In the previous discussion the gradient regulator is related to the second gradient of the plastic strain. To catch the size effect one should include the first order of plastic strain gradient into the constitutive model.

It is known that \( g_1 = \sigma_0 l_1 f_1(\varepsilon^p) \). We set \( f_1(\varepsilon^p) = 1 \) and \( g = 0 \). The flow stress is defined as \( \sigma_y = \bar{\sigma}(\varepsilon^p) + \sigma_0 l_1 |\nabla \varepsilon^p| \). Due to the positive value of \( \nabla \varepsilon^p \), the strength of material is 'hardened' when the strain gradient exists.

Computational micro-hardness, \( H \), is shown in Fig. 5.5 as a function of the indentation depth \( h \). The diagrams are non-dimensionalized by the macro-hardness \( H_0 \) and by \( a_0 \) or \( l_1 \), respectively. The symbols are finite element computations and the solid lines are predictions of Nix and Gao [56]. Significant increase of micro-hardness is restricted near \( h \to 0 \). As in [93] variations about the intrinsic material length in Fig. 5.5(a) can be scaled by the
Figure 5.5: Depth-dependence of the micro-hardness. The symbols stand for computational finite element results. The solid lines are predictions of Nix and Gao [56]. Only the first-order derivative of plastic strain, $|\nabla \varepsilon^p|$, is included in the constitutive equations ($l = 0$). (a) Effects of intrinsic material length $l_1$. (b) Effects of strain hardening exponent $N$.

The present computational results using the first order gradient of equivalent plastic strain agree reasonably with the prediction of Nix and Gao [56], as shown in Fig. 5.5(a). A plot of $(H/H_0)^2$ over $l_1/h$ of Fig 5.6 confirms, furthermore, that this agreement is limited within $l_1/h \leq 6$. Beyond this region the finite element computation under-estimates the micro-hardness, in comparison with Nix and Gao [56]. It is reasonable that with the depth $h$ decreasing, the micro-hardness cannot increase to infinite, as $h \to 0$, and should have a maximum value depending on material length scales, that means, the linear relations between $H/H_0$ and $1/h$ should be satisfied only in an appropriate range. Then gradient plasticity theory, only using the first-order derivative in constitutive formulation can give a reasonable approximation for small $l_1/h$ to the prediction of Nix and Gao [56].

It is interesting to see that in the micro-indentation simulations, the first-order derivative of equivalent plastic strain, $|\nabla \varepsilon^p|$, is more suitable to model the known hardness variations than the Laplacian of plastic strain, $\nabla^2 \varepsilon^p$, whereas in shear band analysis, only $\nabla^2 \varepsilon^p$
5.2.3 Role of the two material length scales

The previous discussions illustrate that modeling with the Laplacian of plastic strain may give a strong effect on micro-hardness variations, while the first gradient of equivalent plastic strain leads to a moderate increasing of the predicted hardness. To fit hardness variations in different materials, it is necessary to adjust both material length parameters. From this point of view, both parameters have to be determined by experimental data.

In Fig. 5.7(a) three curves are depicted with different $l_1$ and $l$ for $N = 1/10$. This figure indicates that to fit the linear relationship, the length scale $l$ is far less than the length scale $l_1$ since $\nabla^2 \varepsilon^p$ has much stronger effects on increasing of micro-hardness. In Fig. 5.7(b) the data are depicted with different $l$ and constant $l_1$ for the same plastic strain exponent.
Results

It shows that using different length scale $l$, the effect of $\nabla^2 \varepsilon^p$ increases or decreases strongly and the micro-hardness deviates gradually from the linear relation. From these figures and numerical calculation we find when $l_1 = 3l \sim 4l$ the computational results do produce the linear relation between $H/H_0$ and $1/h$ over the whole computational range.

![Figure 5.7: Interaction of both intrinsic material length parameters. The symbols stand for computational finite element results. The solid lines denote the least square fitting using a square function. (a) $l = 0.00316a_0$. (b) $l_1 = 0.01a_0$.](image)

5.2.4 Discussions

In this chapter we discussed simulations of micro-indentation tests using the Aifantis gradient plasticity model. Both gradient terms of equivalent plastic strain in the gradient plasticity model are considered.

Computations confirm that the micro-hardness predicted by the gradient plasticity varies with indentation depth, as soon as the gradient regulators differ from zero. Depth-dependence of micro-hardness can be simulated using gradient plasticity models.

Variations of micro-hardness is correlated with the intrinsic material length parameters. In comparison with experimental results of Nix and Co. [56], the Aifantis’ model provides an
overestimate using the Laplacian term of equivalent plastic strain, whereas the first gradient term under-estimates the hardness variations.

Based on extensive computations one can figure out correlation between the intrinsic material length, mechanical property and micro-hardness, as discussed in [93]. Micro-hardness tests provide a method to determine the intrinsic material length in the gradient plasticity models.
Chapter 6

Applications of computational gradient plasticity: Simulation of failure of quasi-brittle materials

The size effect of material strength is well documented for concretes. It has been verified that the mechanical behaviour of concrete ranges from ductile to brittle when the structural size alone is increased and the material and geometrical shape is kept unchanged. Small specimens fail in a ductile manner with slow crack growth. The shape of the load versus displacement response changes substantially according to the variation in size [19]. Therefore it is important to assess the ductility of concrete structures for safety reasons. The gradient plasticity model has been applied for concretes [58]. In this chapter, we focus on the size effect of concrete fracture and the gradient plasticity is applied for the analysis. Here the method of Pamin [58] is summarized and used to analyze the size effect of wedge splitting tests of different sized concrete specimens. Since there is no significant difference between plane strain and plane stress for concrete, plane stress condition is used in this chapter.
6.1 Vertex-enhanced Rankine fracture function

It is well known that the maximum principal stress criterion, i.e., Rankine yield function, can be used for concrete structures. The yield function can be written in the following form:

\[ F = \sigma_1 - \sigma_y (\varepsilon_p, \nabla^2 \varepsilon_p) \tag{6.1} \]

where \( \sigma_1 \) is the maximum principal stress for plane stress condition

\[ \sigma_1 = \frac{1}{2} (\sigma_x + \sigma_y) + \frac{1}{2} \sqrt{\sigma_x^2 + 4\sigma_{xy}} \tag{6.2} \]

For the yield criterion the definition of the equivalent plastic strain rate is

\[ \dot{\varepsilon}_p = |\varepsilon'_1|, \tag{6.3} \]

where \( \varepsilon'_1 \) is the maximum principal plastic strain rate:

\[ \varepsilon'_1 = \frac{1}{2} (\dot{\varepsilon}'_x + \dot{\varepsilon}'_y) + \frac{1}{2} \sqrt{\dot{\varepsilon}'_x^2 - \dot{\varepsilon}'_y^2 - (\gamma_{xy})^2} \tag{6.4} \]

Substitution of the associated flow rule \( \dot{\varepsilon} = \lambda n \) where \( n = \partial F / \partial \sigma \) into (6.4) gives

\[ \varepsilon'_1 = \lambda. \tag{6.5} \]

The Rankine yield criterion is assumed to be activated only when the maximum principle stress, \( \sigma_1 \), is positive. Consequently \( \varepsilon'_1 \) is positive and \( \dot{\varepsilon} = \dot{\varepsilon}'_1 = \dot{\lambda} \). It is clear that in the principle stress plane, the Rankine yield surface for plane stress problems has a vertex if the two principle stresses, \( \sigma_1 \) and \( \sigma_2 \), are positive. It is difficult to deal with the vertex of yield surface by means of gradient plasticity algorithm. As suggested by Pamin [58], the vertex smoothing approach has been used in the region near the vertex. It means that when \( \sigma_1 \) and \( \sigma_2 \) are positive, the new yield function,

\[ F_s = (\sigma^2_x + \sigma^2_y + 2\sigma^2_{xy})^{1/2} - \sigma \tag{6.6} \]

is used to substitute the Rankine yield function 6.1. The corresponding equivalent plastic strain rate, \( \dot{\varepsilon}'_p \) is equal to \( (\dot{\varepsilon}'_x^2 + \dot{\varepsilon}'_y^2 + \frac{\gamma_{xy}^2}{2})^{1/2} \). It assures that \( \dot{\varepsilon}'_p = \dot{\lambda} \). As pointed out by Pamin [58], the use of \( \mu = 0 \) is advantageous to assure the robustness of the algorithm and this assumption introduces a marginal error in the model only. Therefore this vertex-smoothing Rankine yield function is adopted for concrete fracture analysis.
6.2 Softening material curve for concrete

As suggested by Bazant [11], if a continuum formulation based on stress-strain curves with strain softening is to be used, it is necessary to complement it with some conditions that prevent the strain from localization into a region with zero dimension. Such conditions are generally called localization limiters. The model with the simplest localization limiter is the crack band model suggested by Bazant [12]. In this approach, the width of the crack band cannot be less than a certain characteristic value \( h_c \). By introducing

\[
h_c \varepsilon^f = w
\]  

(6.7)

where \( w \) is the cohesive opening displacement, the stress-strain curve for smeared cracking can be written as

\[
F(\varepsilon^f) = f(w) = f(h_c \varepsilon^f)
\]  

(6.8)

where \( f(w) \) is the equation of the softening curve for the cohesive crack model. Consequently there is a unique relationship between the crack band model and the cohesive crack model.

As suggested by Aifantis, the flow stress in gradient plasticity theory is

\[
\bar{\sigma}_g(\varepsilon^p) = \sigma(\varepsilon^p) - g \nabla^2 \varepsilon^p
\]  

(6.9)

and the yield function is:

\[
F = \Phi(\sigma) - \bar{\sigma}_g(\varepsilon^p, \nabla^2 \varepsilon^p) = 0
\]  

(6.10)

From the 1D shear band analysis, de Borst and Mühlhaus [24] derived that the width \( h_c \) of a shear band and the intrinsic length \( l \) suggested by gradient plasticity can be linked by the following relationship

\[
h_c = 2\pi l
\]  

(6.11)

and the coefficient \( g \) then is

\[
g = -\sigma^\prime(\varepsilon^p)l^2
\]  

(6.12)

where \( \sigma^\prime(\varepsilon^p) \) is the derivative of the stress-strain curve \( \sigma(\varepsilon^p) \). In [25], these relations are applied to concrete fracture.

For all points in the cracking band, when \( \sigma(\varepsilon^p) \) decreases to zero, the nonlocal stress \( \bar{\sigma}_g(\varepsilon^p, \nabla^2 \varepsilon^p) \) should decrease to zero too, otherwise the crack cannot propagate when the
Simulation of failure of quasi-brittle materials

A gradient plasticity model is used. Since the Laplacian term $\nabla^2 \varepsilon^p$ can be negative or positive, $g$ should not be a constant as has been assumed in ductile material analysis. In concrete structures, the Eqn. (6.12) suggested by de Borst et al. is used in this chapter. That means nonlinear strain-softening curves can be selected only since $\bar{\sigma}(\varepsilon^p)$ will be constant when linear or bi-linear strain-softening curves are selected. Hence a nonlinear strain-softening curve should be used for the computation and in this way crack propagation can be simulated.

Here the Cornelissen-Hordijk-Reinhardt curve [36] which was formulated originally in the context of cohesive cracking is adopted. The choice is suggested by Pamin [58]. In his work of gradient plasticity he has re-written the function in continuum format:

$$\bar{\sigma}(\varepsilon) = f_t \left[ 1 + \left( c_1 \frac{\varepsilon^p}{\varepsilon_u^p} \right) \exp \left( -c_2 \frac{\varepsilon^p}{\varepsilon_u^p} \right) - \frac{\varepsilon^p}{\varepsilon_u^p} (1 + c_1^3) \exp \left( -c_2 \right) \right], \quad (6.13)$$

where $c_1 = 3.0$, $c_2 = 6.93$; $f_t$ is the uniaxial tensile strength and $\varepsilon_u^p$ is the ultimate value of the equivalent fracture strain. The relation between the curve and the fracture energy $G_f$ is assumed to be

$$\varepsilon_u^p = \frac{5.14G_f}{h_c f_t}. \quad (6.14)$$

The general form of the yield function is shown in Fig. 6.1.

---

**Figure 6.1:** Nonlinear softening for concrete under Mode-I fracture (cf. Hordijk [36])
6.3 Application to concrete fracture: wedge splitting test

6.3.1 Experimental results

The performance of stable fracture mechanics tests on concrete specimens is difficult due to the small deformations at rupture of concrete and the stiffness of concrete specimens compared to the stiffness of the testing machine. The wedge splitting test overcomes these difficulties. A schematic illustration of the test set-up is given in Fig. 6.2. Two wedges are pressed symmetrically between four roller bearings under controlled condition in order to split the specimen into two halves. The test set-up is similar to the one as described in RILEM recommendation AAC 13.1 (1994). The crack mouth opening displacement (CMOD) at both sides of the specimen at the level of the loading points, and the applied vertical load $F$ can be measured [81]. From the measured vertical load and the known wedge angle the horizontal splitting force is calculated. The measured CMOD is the mean value of the two displacement transducers on the two opposite sides of the specimen. All tests are run under

Figure 6.2: Schematic representation of the wedge splitting test: a). specimen on 2 linear supports. b). displacement transducers on both sides of the specimen. c). steel loading devices with four roller bearings. d). load introducing traverse with wedges
CMOD control. The geometrical data are listed in Fig. 6.3 and Table 6.1. Experimental results will be compared with numerical predictions.

![Figure 6.3: Geometry of the wedge splitting specimens](image)

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Table 6.1 Geometrical data of wedge splitting specimens

In order to determine numerically the non-linear fracture mechanics parameters from experimental results of specimens with similar geometry but different size, a cohesive model
6.3. Application to concrete fracture: wedge splitting test

Figure 6.4: Mean load deformation curves and numerical simulations for all normal concrete specimens from [79], [81]

Based on a nonlinear finite element program SOFTFIT earlier developed at ETH has been used to determine the strain softening diagram as a bilinear function by inverse analysis. The experimental and numerical data from [81] are listed in Table 6.2 and Fig 6.4. In [81] similar results obtained on specimens prepared with hardened cement paste, mortar and dam concrete can also be found. In this chapter, the task is to apply gradient plasticity theory to the numerical analysis of concrete specimens and to try to reproduce the size effect which has been found in experiments. Therefore we will use both the experimental and numerical data from [81] as the initial input data for gradient plasticity modeling.

<table>
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<td>$F_{sp}^{max}$ [kN]</td>
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<td>47.52</td>
<td>86.49</td>
<td>167.32</td>
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<td>$G_f^{exp}$ [N/m]</td>
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<td>196</td>
<td>244</td>
<td>303</td>
<td>369</td>
<td>322</td>
</tr>
<tr>
<td>$G_f^{num}$ [N/m]</td>
<td>156</td>
<td>188</td>
<td>251</td>
<td>297</td>
<td>387</td>
<td>340</td>
</tr>
<tr>
<td>$f_t$ [N/mm$^2$]</td>
<td>2.43</td>
<td>3.36</td>
<td>2.42</td>
<td>2.10</td>
<td>1.95</td>
<td>2.5</td>
</tr>
</tbody>
</table>

Table 6.2 Experimental data obtained by wedge splitting tests (normal concrete) [81]

From Table 6.2 and Fig. 6.5 it is found that uniaxial tensile strength is not constant,
but decreases gradually with an increase of specimen sizes. This can be explained by Weibull theory. The size effect of fracture energy is obvious: fracture energy increases with the increase of size of specimens and finally reaches a constant value. In [79, 80], the dependence of the specific fracture energy $G_f$ of specimens with equal size is also given as function of the maximum aggregate size $\Phi_{\text{max}}$. The observed fracture energy increases with maximum aggregate size. This means that the ductility of the material increases with maximum aggregate size $\Phi_{\text{max}}$.

### 6.3.2 Numerical simulations

In the FE simulations using gradient plasticity, we assume Young's modulus $E = 31500 N/mm^2$ and Poison ratio $\mu = 0.2$ for the elastic region and $\mu$ is forced to become 0 in the plastic region as suggested by Pamin [58]. The nonlinear softening stress-strain relation is given by Eqn. (6.13). The value of material length $l$ is in the range of 1 mm - 8 mm as suggested by Pamin [58]. Therefore the corresponding width of fracture process zone is between 6.5 mm and 50 mm if Eqns. (6.7), (6.11) are used.

To simulate the crack propagation and to find the influence of strain gradient on the size effect on strength, one half of the wedge splitting specimens is discretized using 8-nodal
6.3. Application to concrete fracture: wedge splitting test

Figure 6.6: a). Undeformed mesh of wedge splitting specimen. b). Final incremental deformation of the configuration
elements. The initial mesh and its mesh distortion are shown in Fig. 6.6. The gradient plasticity model is used in the fine mesh area near the notch only and the conventional elastic model is used in the area far from the notch. It is clear that using gradient plasticity the fracture zone is not limited to one layer of elements but it is rather distributed to the neighboring elements due to the gradient effects. To simulate the experiments, displacement control is used in the numerical analysis.

In the gradient plasticity model we need to assume the tensile strength $f_t$ and the fracture energy $G_f$ or we have to determine these values by inverse analysis. The corresponding ultimate equivalent fracture strain is derived from Eqn. (6.14). From Fig. 6.5 it is found that the values of fracture energy and tensile stress are not constant. $f_t = 2.5 N/mm^2$ and $G_f = 345 N/m$ are realistic values for specimens with a height $H = 1600 mm$ or larger, while $f_t = 2.75 N/mm^2$ and $G_f = 275 N/m$ are good assumptions for specimens where the height $H$ is $400 mm$. To analyze the effect of material length $l$, different length values, $l = 1 mm$, $l = 6 mm$ and $l = 8 mm$, are selected. The simulated Loading-CMOD curves of different sized specimens using three different material lengths are shown in Fig. 6.7. It is shown that the Loading-CMOD curve is not strongly influenced by the material length. This phe-
Simulation of failure of quasi-brittle materials

Figure 6.7: The influences of different material lengths \( l \) on load-CMOD curve for different sized specimens. a). \( H=400 \text{mm} \) b). \( H=1600 \text{mm} \)

nomenon has also been found by Pamin [58]. The reason is that in this case the fracture energy is a material constant and governs the softening process. Therefore the observation is important if one considers the problem of experimental determination of length scale as a material parameter. It seems that the material length influences the deformation pattern and the distribution of fracture strains only, but it does not influence the load-displacement relation since the released energy does not change. It seems that to obtain mesh-objective results any non-zero value of material length within a recommended region can be assumed. This is quite different from ductile materials such as steel. Fig. 6.7 verifies that gradient plasticity model if applied to concrete-like composite materials can supply mesh-independent results.

From the analysis of experimental data shown in Fig. 6.5, it is obvious that if the specimen is big enough, fracture energy and tensile strength can be considered to be constant [81]. The width of the fracture process zone for normal concrete is around 50 \( mm \) [80]. Hence it is reasonable to assume that fracture energy \( G_f \), tensile strength \( f_t \), and the width of fracture zone are material constants when the height of a given specimen is at least 1600 \( mm \). In order to check whether or not the fracture energy is constant numerical simulation of CMOD-curve has been carried out using the gradient plasticity model. The material
parameters, $f_t = 2.5N/mm^2$ and $G_f = 345N/m$, are used for all specimens with different size ($H = 100 - 3200 mm$). To analyze the relation between size effect and material length, a unique stress-strain curve should be applied. Therefore $l = 8 mm$ is a realistic choice. The results of numerical simulations are shown in Fig. 6.8 and Table 6.3. It can be seen that the assumptions of $G_f$ and $f_t$ is realistic for large specimens but lead to too ductile Load-CMOD curves for small specimens.

Figure 6.8: Numerical simulations of Mean load-deformation curves for all normal concrete specimens.

<table>
<thead>
<tr>
<th>Height [mm]</th>
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<td>$F_{s p}^{max}$ [kN]</td>
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<td>26.12</td>
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<td>$G_f^{num}$ [N/m]</td>
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<td>260</td>
<td>280</td>
<td>288</td>
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<td>286</td>
</tr>
</tbody>
</table>

Table 6.3 Results of numerical simulations with $f_t = 2.5N/mm^2$ and $G_f = 345N/m$

One reason for the fact that the calculated $G_f$ from numerical simulations is smaller than the assumed $G_f$ which is introduced by the stress-strain equation (6.13) is that the long tail of stress-CMOD curves can not be captured due to numerical difficulties. Another reason is that the width of the fracture process zone (Eqn. (6.7)) is not accurate when a nonlinear stress-strain curve is used in analysis because Eqn. (6.11) is derived from 1D shear band analysis and a linear stress-strain curve is assumed. It is known that the strain is not
constant in the fracture process zone. Therefore Eqn. (6.11) will lead to a larger width of
the process zone and the assumed fracture energy is higher than the calculated one.

![Figure 6.9: Numerical simulations of nominal stress-strain curves for all normal concrete
specimens.](image)

To check the brittleness of the descending branch, the nominal stress \( \sigma_m = \frac{F_p}{H_L t} \) and
the nominal strain \( \alpha = \frac{CMOD}{H^*} \) are introduced. \( H_L, t \) and \( H^* \) are shown in Table 6.1 and
Fig. 6.3. The results are shown in Fig. 6.9. It can be seen from the descending branch
that the brittleness of the tested specimens increases with increasing specimen size. The
nominal peak stress increases with decreasing specimen size. The characteristic size effect as
observed by testing of brittle solids is obvious: the bigger the size of the specimen, the lower
the failure load will be. It verifies that the mechanical behaviour of concrete ranges from
ductile to brittle when the structural size is increased and both the material and geometrical
shape are kept unchanged.

### 6.3.3 Discussion

The conclusion from Fig. 6.7 and 6.8 raises some doubts. The question here is: Is it true
that the size effect of fracture energy can be captured by the gradient plasticity model? It
is said in the gradient plasticity theory that the increase of material length \( l \) does increase
6.3. Application to concrete fracture: wedge splitting test

the material strength (load carrying capacity) of ductile materials. Fig. 6.9 also shows the size effect of the peak stress and strain softening branch for concrete. For ductile materials, the material parameters can be given from stress-strain curve and this curve is uniquely determined from experimental data of the tension test when specimens are smooth and large enough. However the stress-CMOD curve is more often determined for concrete materials. In gradient plasticity, \( G_f \) and \( f_t \) have to be assumed before the calculation and a realistic stress-strain curve is necessary. Different material lengths lead to different ultimate fracture strain \( \varepsilon_f^u \) in Eqn. (6.14). It means that different stress-strain curves derived from Eqn. (6.13) are used for different material lengths. Fig. 6.7 verifies that when \( G_f \) is assumed to be constant, if different material lengths, i.e. different stress-strain curves are used, almost the same load-CMOD curve is obtained. The length scale introduced by the gradient plasticity theory does not change the value of the fracture energy, but it determines the width of the fracture process zone.

![Figure 6.10: Numerical simulations of Mean load - CMOD curves with different values of \( G_f \) and \( f_t \)](image)

In [58], the gradient plasticity model is applied to direct tension tests of concrete. The width of the fracture band is assumed to be equal for all specimens with different size due to the introduction of material length \( l = 2 \, mm \). The size effect in both the peak stress and strain softening response of nominal stress - average strain curve has been observed [58]. However, no strong size effect of nominal stress - displacement curve can be captured.
because the fracture energy is set to be constant. That means that the computational results guarantee that the fracture energy is a constant.

From Fig. 6.8, it can be seen that when the height of an element is at least 1600 mm, the set of material parameters $G_f = 345 N/mm$, $f_t = 2.5 N/mm^2$ and $l = 8 mm$ gives reasonable numerical simulations of the load-CMOD curve data for large specimens. The computational results fit experimental data well. It is usually assumed that the value of computational fracture energy does not change when the gradient plasticity model is used. However, the experimental results supply evidence that the fracture energy is a function of the size of specimens (Fig. 6.5). Therefore, to capture the size effect of fracture energy which has been supplied from experiments (Table 6.2 and Fig. 6.5), different values of $G_f$ and $f_t$ should be assumed for smaller specimens. Fig. 6.10 gives computational results for several specimens using different values of $G_f$ and $f_t$ which are taken from the fitted data in Fig. 6.5. The results in Fig. 6.10 show clearly that the size effect of load-CMOD curves can be simulated by gradient plasticity model when fracture energy and tensile strength are introduced in a realistic way.

It can be concluded that gradient plasticity model can describe the size effect of peak stress (load carrying capacity) and strain-softening if the size dependence of fracture energy and tensile strength are introduced in a realistic way. The failure of concrete changes from ductile to brittle when the size of an element increases. However, the relationship between the internal length scale and the fracture energy can not be determined at this moment. This point should be further considered.
Chapter 7

Applications of the nonlocal damage model: failure analysis of ductile materials

There are more and more experimental indications to show that fracture mechanics parameters depend on both specimen size and geometry. In investigating the size dependence of fracture mechanics parameters, the size and geometry of specimens should be carefully considered. If the size of a structural element is comparatively small with respect to the maximum heterogeneity of the material, the heterogeneity of the material's structure should be taken into account [79, 80]. It is interesting to find and quantify the size and scale effects of fracture mechanics. In the EU research project REVISA extensive experiments of a reactor pressure vessel steel 20MnMoNi55 have been performed in Paul Scherrer Institute to find the size effects in plastic flow and failure [42, 43, 44]. To simplify data processing and computations, the specimen geometries are restricted in most conventional tension and bending. Specimens with and without notches in scaled dimensions are tested in detail to characterize the influence of specimen size, strain rate and strain gradients on plastic flow and failure. The characteristic sizes of the specimens vary from 3 mm up to 140 mm and the geometry factor is up to 10 for each sort of geometry configuration. In this section the nonlocal damage model is used to investigate the geometry dependence of the plasticity
behaviour and material failure, and to fit the experimental work.

For engineering materials stress-strain relation is determined from the uniaxial tension. The relation of the matrix stress and strain is assumed power-law hardening. The present steel reveals a considerable Lüder band and significant strain hardening after yielding. From uniaxial tensile tests, the stress-strain curve is assumed as:

\[
\epsilon = \begin{cases} 
\frac{\sigma}{E} & 0 \leq \epsilon \leq 0.002 \\
\sigma_0 & 0.002 < \epsilon \leq 0.01 \\
\frac{\alpha \sigma_0}{E} \left( \frac{\bar{\sigma}}{\sigma_0} \right)^{1/n} & \epsilon > 0.01
\end{cases}
\]  

(7.1)

where Young's modulus \( E = 500\sigma_0 \), \( \alpha = 2.5 \), \( \sigma_0 = 435\text{MPa} \). The exponent \( n \) is fitted to 7.25.

Constitutive parameters \( q_1 \) and \( q_2 \) in the GTN model are fitting parameters. Studies of Koplik and Needleman [41] found out that \( q_1 = 1.0 - 1.5 \) and \( q_2 = 1 \) are a good choice for ductile solids. In our study we set \( q_1 = 1.5 \), \( q_2 = 1 \). Zhang [95] reveals that effects \( f_0 \) and \( f_N \) in the GTN model are computationally analogous. One cannot uniquely separate the parameter \( f_0 \) from \( f_N \). In this study it is found that the void nucleation is secondary in comparing with void growth due to high plastic deformations. The initial damaged material behaviour can be characterized by \( f_0 \) value. Hence the initial void volume fraction \( f_0 \) is set to 0.001. The critical void volume for coalesce \( f_c \) is 0.01. The void volume fraction at final failure of the material \( f_f \) is assumed to be 0.15 and \( f_u^* = 1/q_1 \). The intrinsic length scale \( l \) in the nonlocal damage model acts as a fitting parameter here. From computations for all sorts of specimens it is found that the length scale of about 0.2 mm - 0.3 mm fits the experimental data of tensile specimens reasonably. In the present study we set \( l = 0.24 \text{ mm} \). Here \( l \) acts as a fitting parameter of experimental results although \( l \) is much larger than the size of voids. The real range of material length \( l \) need more theoretical and experimental studies in the future.
7.1 Uniaxial tension specimens

Three groups of size-different but geometry-similar tension specimens (R1, R2, R3) have been investigated (Fig. 7.1). The diameters of the specimens are 3 mm, 9 mm and 30 mm, respectively. The measuring length of specimens is 6 times more than the corresponding diameter. To study efficiency of the nonlocal damage model, we use a single finite element mesh (200 elements) which is fine enough for each type of specimens as shown in Fig. 7.2.

To generate a concentrated necking at the symmetric cross-section of the uniaxial tension specimens, we introduce a local geometric defect, i.e. the radius at the symmetric section is 0.5% smaller than the overall radius. The geometric defect does not affect the necking but strength of the specimen slightly. A variety of specimens tension are tested at room temperature under quasi-static loading conditions. In Fig. 7.3 a specimen of type R3 after fracture is shown to demonstrate the shape of local deformation. Computational and experimental results are plotted in Fig. 7.4 and 7.5. In Fig. 7.4a the engineering stress vs. elongation and in Fig. 7.4b the engineering stress vs. necking are shown. The relation of two deformation components, i.e. elongation vs. necking, is given in Fig. 7.5. The symbols represent the experimental results for the three size-different groups of specimens and the lines are the computational predictions. The results of two specimens for each
Figure 7.2: Finite element meshes for axisymmetric specimen. Due to symmetry only a quarter of the specimen is discretized. The mesh for smooth round bar contains 200 elements. The specimen is loaded only at the upper edge.

Figure 7.3: Example of the experimental tests. The numbers within the circles denote the radii of the circles, while the number near the smallest cross-section of the specimen denotes the smallest diameter during necking. Specimen R3009, strain rate $10^{-3}/s$
Uniaxial tension specimens

Figure 7.4: Comparisons of experimental with computational results for three groups of smooth round specimens R1, R2 and R3. Each group contains two specimens summarized in the diagrams. (a): Mean stress vs. elongation; (b): Mean stress vs. necking at the fracture cross section.

Group are selected in these figures. The present reactor pressure vessel steel is highly ductile and deformations around the necking develop rather uniformly, so that the actual loading capacity decreases gradually. From the experimental data in Figs. 7.4 and 7.5, the evolution of damage does not affect the stress vs. elongation curves up to the maximum stress point. No size effect is obtained till the maximum stress point is reached. Also for the ultimate tensile strength no significant influence of size can be derived. Our computations confirm that the yield stress and the pre-necking behaviour of material is not influenced by the size due to small strain gradients. Only in the post-necking region, the load capacity of small specimens is slightly stronger than that of the large and medium specimens (R3 and R2) with increase of strain gradients. The elongation and the necking (reduction of cross-area diameter) show only a slight decrease with size increase, in agreement with experimental results.

Fig. 7.6 shows the distributions of damage evolution at the symmetric cross-section.
Figure 7.5: Correlations of the elongation and necking. The symbols are experimental records, lines computational results.

Figure 7.6: Distributions of damage evolution along the axisymmetric cross section; The radius is normalized by initial radius of specimen; (a) Large specimen D=30 mm; (b) Small specimen D=3 mm.
7.2 Round-notched tension specimens

A notch in a tension specimen changes stress triaxiality significantly. In a notched specimen the strain concentration occurs much earlier than the smooth one. Three groups of size-different but geometry-similar tension specimens with round notches (T1, T2 and T3) are studied (Fig. 7.7). The diameters of the specimens are 3 mm, 9 mm and 30 mm, respectively. The radii of notches are 0.3 mm, 0.9 mm and 3 mm respectively. The measuring length of specimens is 6 times more than the corresponding diameter. The finite element mesh for notched specimens is in Fig. 7.8.

In Fig. 7.9a the engineering stress vs. elongation curves and in Fig. 7.9b the engineering stress vs. necking curves are plotted. The symbols represent the experimental data and the lines the FE simulations. The experimental observations show that material strength
and failure are related to the size of specimens. By integrating the strain gradient of the specimens into the flow stress, the strength of specimens increases and the material failure is delayed significantly with decrease of the sizes. The initial yield stress and the pre-necking behaviour do not change due to small strain gradients, which are in agreement with the experiment results. For the large specimens T3, the computational results meet both axial and radial deformations reasonably. For the medium specimens T2, experimental results show almost no size effect on the stress vs. elongation relation, but the diameter reduction is slightly larger than that of T3. Our computational simulations give reasonable stress vs. elongation fitting but the diameter reduction is smaller than that of experimental records. For small specimens T1, the FE simulation for the stress-elongation data is suitable. The strength of the material is 'hardened' and the fracture point is well determined by computation. The diameter reduction of FE simulation is slightly smaller than the experimental results but still acceptable compared with the experimental results in Table. 7.1. In Fig. 7.10 the elongation vs. necking diagram is shown. In the post-necking region, the relation between elongation and necking is well fitting. The local deformation shows a clear size
Figure 7.9: Comparisons of experimental with computational results for three groups of notched specimens T1, T2 and T3. There are two specimens results in the diagrams for each group. (a): Mean stress vs. elongation; (b): Mean stress vs. necking at the fracture cross section.

Due to effects of strain gradients and intrinsic length scale, the deformation around the notch is more 'homogeneous'. With the same elongation for different sized specimens, the smaller specimens has a smaller necking than the bigger one.

It is reported in [43] that a semicircle notch remains its shape (Fig. 7.11). Starting with a real semicircle the notch opening becomes a chord of segment of a circle. The notch shape at fracture is a segment of a circle. In Fig. 7.12 the local deformation near notch at fracture for the three different specimens T1, T2 and T3 is plotted. Computation reveals that the deformed notch in the present specimen remains almost a co-axial circle of initial notch. For smallest specimens T1, the notch opening and necking is larger than that of large specimens.

Fig. 7.13 shows the damage evolution and plastic strain evolution along the axisymmetric cross section for T1 and T3 specimens, respectively. In Figs. 7.13a and 7.13c it is confirmed that the voids grow rapidly at the center of specimens where the hydrostatic
Figure 7.10: Correlations of the elongation and necking. The symbols are experimental results, lines computational predictions.

Figure 7.11: Example of a notched specimen (T3017) at fracture. The numbers with the circles exhibit the radii of the circles, while the number near the smallest cross-section of the specimen denotes the smallest diameter during necking.
stress is high. The void distribution for small specimens T1 is smoother than that of large specimens T3. In Figs. 7.13b, d the evolution of effective plastic strain is plotted. The maximum effective plastic strain is concentrated around the notch. At the beginning the distribution of plastic strain for both small and large specimens are similar due to small plastic strain gradients. With the increase of deformation and damage formation, the effect of intrinsic length scale becomes important. The influence of the length scale leads to a more 'homogenized' deformation for the small specimen. This figure demonstrates that the gradient plasticity doesn’t change the failure pattern and deformation characteristics for the size-different specimens but 'strengthen' the material and make the deformation field more homogeneously.

In Table 7.1, the diameter reduction and notch opening for both experimental tests and FE computations are summarized. The FE computations with the nonlocal damage model give reasonable notch opening displacement (NOP) for T1 and T3. For T2, the computational result is slightly smaller than the test. The FE simulations of diameter reduction for all three groups are in the scatter band of experimental results. Only for T1 specimens the computation is less than 10% smaller. The computations of local deformations in the notch area show that the nonlocal damage model fits the experiment results well. The size effects of local deformations observed from experiments, i.e. the reduction of diameter and increasing of NOP with the decrease of size, are well captured by the nonlocal damage model.
Figure 7.13: The distribution of damage and effective plastic strain evolution along the axisymmetric cross section; The X co-ordinate is the normalized radius; (a): damage evolution of large specimens T3, D=30 mm (b): plastic strain evolution of large specimens T3, D=30 mm (c): damage evolution of small specimens T1, D=3 mm (d): plastic strain evolution of small specimens T1, D=3 mm
Table 1: Experimental and computational results of the local deformation parameters

<table>
<thead>
<tr>
<th></th>
<th>Diameter Reduction</th>
<th>Notch Opening Displacement</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( (R_0 - R)/R_0 \times 100% )</td>
<td>( U_{\text{notch}}/r_0 )</td>
</tr>
<tr>
<td></td>
<td>Experiments</td>
<td>FE simulation</td>
</tr>
<tr>
<td>small specimens T1</td>
<td>40% - 52%</td>
<td>42%</td>
</tr>
<tr>
<td>medium specimens T2</td>
<td>30% - 40%</td>
<td>36%</td>
</tr>
<tr>
<td>large specimens T3</td>
<td>30% - 35%</td>
<td>35%</td>
</tr>
</tbody>
</table>

\( R_0 \): initial radius of specimen, \( r_0 \): initial radius of notch

7.2.1 Predictions of the size effects from computations

From the computations, the nonlocal GTN model can fit the experimental results well for the three groups of notched specimens. It is interesting to use the model to analyze the size effects of material failure for a wider range of specimens’ sizes. In Fig. 7.14 the size effects of material strength and deformations are plotted for different specimens. The diameters of specimens vary from 1.25 mm to 20 mm. It is confirmed that the material is strengthened and the material failure is delayed with the decrease of the specimen’s size. From the analysis of Fig. 7.14, the size-dependent local deformations at fracture are summarized in Fig. 7.15. It shows that the intrinsic lengths of material has almost no influence on the material failure for the specimens which diameter is larger than 4 mm. For the specimens which diameter is smaller than 4 mm, the elongation, necking and notch opening at fracture increase dramatically. The normalized size effects of elongation, necking and notch opening are drawn in Fig. 7.15d. Due to the strain concentration around notch area, the size effect of notch opening is more significant than the size effect of elongation. From Fig. 7.15d it is obvious that size effect of notch opening is much stronger than the size effect of necking at notch area. Therefore the notch opening is very appropriate to measure the size effects of local deformation for tension tests with notch.
Figure 7.14: Computational predictions for different specimens; the diameter of specimens is from 1.25 mm to 20 mm.
Figure 7.15: Computational predictions of the deformations at fracture depending on size of specimens. (a): elongation (b): Necking (c): Notch opening (d): normalized size effects at fracture.
In this chapter only Laplacian term is used. As pointed out in chapter 5, only considering the Laplacian term of plastic strain into constitutive law, may overpredict the size effect of material deformation at failure with the significant decrease of specimen’s size. If the size effect of material strength changed smoothly with the change of the size, the first gradient term, $|\nabla \varepsilon^p|$, may be taken into account.

It is reasonable that the critical deformations at fracture cannot increase to infinity when the size of specimen decreases to infinity. As mentioned in chapter 2, the intrinsic length scale should be a measurement of the microstructure of material. Therefore the length scale should be useful only in some appropriate range in which the size of microstructure is still small comparing with the size of the material’s structure.

### 7.3 Notched bending specimens

Three groups of size-different but geometry-similar three-point bending specimens (S1, S2, S3) with U-form notches have been investigated. The specimens are 140mm, 25mm and 10mm wide (H), respectively. The lengths (L) are 770mm, 137.5mm, 55mm and the notch radius (r), are 14mm, 2.5mm, 1mm, respectively. The depth of notch is 3r for all the three groups of specimens. Due to symmetry only one half of the specimens is used for modeling. The finite element mesh used for computation and the mesh distortion are plotted in Fig. 7.16. The length between the two rigid circular supports are defined as $S = 2H$. The upper rigid support is fixed during deformations and the radius of it is 0.4H. The radius of the lower circular support at loading point is 0.5H. Frictionless contact between supports and specimen is assumed during loading process. To analyze the size effect in material failure, the bending strength is defined as

$$\sigma = \frac{F}{A}$$  \hspace{1cm} (7.2)

where $F$ is the load on the specimen, $A = (H - 3r)t$ is the area of cross section ahead of the notch and $t$ is the thickness of specimens. The bending angle $\alpha$ can be expressed as

$$\alpha = \arctan \left( \frac{2v_x}{S} \right) + \frac{180}{\pi}$$  \hspace{1cm} (7.3)

where $v_x$ is the x-direction displacement of the lower rigid support.
7.3. Notched bending specimens

Figure 7.16: Finite element mesh for three-point bending tests. a). 1050 elements are used. b). the deformation of the bending specimen.

Experimental results and numerical predictions of conventional 2D and 3D GTN damage model are plotted in Fig. (7.17a). From the study of 3D experiments, it is known that the crack initiates at the center of the notch and propagates gradually and slowly, in both thickness and ligament directions. It results in that the bending strength can not decrease rapidly since the strength capacity does not exhausted immediately. Strong necking around notch help to arise the bending strength of specimen furthermore. It can be found in Fig. (7.17a) that the bending strengths of both experiment result and numerical simulation have no dramatic decrease due to slow crack propagation. In the present computation plane strain assumptions are used. However, the plane strain assumptions give strict restraint along the Z direction. When crack is formed at the center of the notch, the material at the damage region lose strength capacity in the whole front area due to 2D assumption. The crack will propagate uniformly along ligament direction. It follows that the bending strength decreases rapidly. The difference between 2D and 3D simulations shows that 2D model is not suitable to simulate the seen 3D crack propagation.

Although accurate numerical analysis of the bending tests needs 3D gradient plasticity
Figure 7.17: Comparisons of experimental with computational results for three groups of notched specimens S1, S2 and S3. There are two specimens results in the diagrams for each group. (a): Experimental results and numerical results of conventional Gurson damage model; (b): Experimental results and numerical results of nonlocal Gurson damage model models, in this part we only check whether or not the nonlocal GTN damage model based on gradient plasticity theory can capture the size effects in crack initiation in bending configuration. Therefore the plane strain version of the nonlocal damage model is used here. In the bending simulations, all material and damage parameters used in tension tests are still applied.

In Fig. (7.17), the experimental results show strong size effect of bending strength for size-different specimen. The 2D computational results using the nonlocal damage Gurson model has been plotted in Fig. (7.17)b. The scattering of these curves is due to the discretisation of contact area in the commercial program ABAQUS. Computational results show that the size effect is very weak between the largest and smallest specimens. The reason is that the strain gradients in 2D simulation is smaller than the realistic 3D strain gradients since under plane strain condition $\varepsilon_{zz}$, $\varepsilon_{xx}$ and $\varepsilon_{xy}$ are assumed to be zero. Therefore using 2D model the increase of bending material is smaller than the observation from experimental results.
7.3. Notched bending specimens

To realize stronger size effect for the bending strength, two smaller specimen, S4 and S5 are used in 2D nonlocal computation. The widths H are 5mm and 2mm for S4 and S5, respectively. The corresponding lengths are 27.5mm and 11mm respectively. The bending strength vs. bending angle curves for S1, S2, S3, S4, S5 are plotted in Fig. (7.18)a. The strength of S4 is obviously larger than that of S1, S2 and S3. The strength of S5 is strongly larger than all the others. To analyze the size dependence, the bending strength of different specimens at the bending angle $\alpha = 30^\circ$ are drawn in Fig. (7.18)b. For the specimens which width are less than 10mm, the bending strength increases significantly. This figure is similar to Fig. (7.15). It is clear that the strength increases fast when the size is less than the threshold for 2D plane strain assumptions. The size effects of bending strength can be investigated by the nonlocal GTN model based on gradient plasticity although the numerical results of 2D model deviate from the 3D experimental results.
Chapter 8

Conclusions and outlook

In the dissertation, a new algorithm of computational gradient plasticity on finite strain assumptions is formulated. Based on the new algorithm of gradient plasticity, the formulation and finite element implementation of a micro-mechanical damage model by implementing gradient plasticity theory into GTN damage model is presented. In this model, the matrix material is gradient-dependent and the shape of the constitutive equation is not changed. Results confirm that the algorithm is suitable for computing the strain-softening problem. Shear band analysis shows that the width of shear band is uniquely determined by the material length scale parameter, not by the geometry factors.

Due to the introduction of material intrinsic length into constitutive relationship, the size effects of material can be investigated by the gradient plasticity theory and mesh-dependence of computational results can be eliminated. In the dissertation several applications to the investigation of size effects phenomena are performed. The simulations of micro-indentation using Aifantis’ gradient plasticity theory are discussed. Computational results confirm that the micro-hardness predicted by the gradient plasticity varies with indentation depth, as soon as the gradient regulators differ from zero. Depth-dependence of micro-hardness can be simulated using gradient plasticity models. Micro-hardness tests provide a method to determine the intrinsic material lengths in the gradient plasticity model. The size effects of concrete material is investigated. It is turned out that the mechanical behaviour of concrete ranges from ductile to brittle when the size of structure is increased.
along without the change of shape of geometry.

Computational analysis of ductile material failure shows that a mesh-independent solution can be achieved by the micro-mechanical damage model. The result that increase of the material strength will delay the computational material failure time is consistent to the known experimental results in ductile materials. Computational analysis of ductile failure in notched specimens shows that the size effects observed from experiments are predicted by the intrinsic length scale introduced into gradient plasticity model. The nonlocal GTN damage model based on gradient plasticity has the potential for the assessment of material failure and provide reliable explanation for the size effects of material behaviour.

As discussed in the dissertation, The physical meaning of the additional boundary conditions is still an open issue. Delicate considerations and discussions of boundary conditions should be investigated from thermodynamical approach.

Although $C^1$ continuous interpolation method has its own advantages, the mesh topology has some limits and 3-D formulation and simulation is still unreachable due to the difficulty of the requirement of high order continuity. In order to capture the size effects of material behaviour accurately in some cases, i.e. 3 point bending tests of ductile material, 3D model is necessary. Therefore 3D gradient plasticity model should be considered. At the one hand, New interpolation method for finite element implementation should be taken into account, at the other hand, the nonlocal damage model based on gradient plasticity may be implemented into other numerical methods, i.e., meshfree methods. In the commonly used approximation theories for meshfree discretization, non-locality is embedded in the weight function. The support size of the weight function is usually greater than the nodal spacing and therefore the approximation is inherently non-local. Hence it is attractive to embed gradient-type plasticity theory and micro-mechanical damage model into meshfree methods.
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