MICROMECHANICAL MODEL FOR DAMAGE AND FAILURE OF BRITTLE MATERIALS: APPLICATION TO POLYCRYSTALLINE ICE AND CONCRETE

by

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Abstract

A micromechanical model is developed to predict the failure strength of polycrystalline ice in the brittle region. Final failure is predicted when the stress field at the tip of one or more of the nucleated cracks satisfy the maximum principal stress criterion. The micromechanical damage model is used to investigate the statistical effects caused by the randomness in the microstructural properties. A probability theory is used to formulate the probabilistic distribution of the failure stress and the compliance caused by the distribution of the underlying microstructural parameters. The failure stress and specimen size effect of a finite sized polycrystalline material are predicted by a micromechanical model. The model takes into account the interaction between microcracks and between microcracks and specimen boundary in the computation of the stress field and subsequently of the unstable propagation of microcracks. A micromechanical model is applied to predict the behavior of polycrystalline ice in the ductile to brittle transition domain. The maximum principal tensile stress criterion is used to decide the nucleation of wing cracks.

The constitutive relation of plane concrete is predicted using a micromechanical model. An initial defect is assumed to exist in the aggregate-hardened cement paste interface. When the maximum principal stress fracture criterion is satisfied the pre-existing defects nucleate into bond cracks along the interfaces which have smallest fracture toughness. Once the bond cracks are formed they grow into mortar as the loading increases. The overall compliance is calculated from the damage due to microcracks, and the predicted stress-strain curves are compared with experimental data.

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To my parents
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INTRODUCTION

1.1 Research in constitutive mechanics

The laws of force and momentum balance are common to most bodies in nature. These laws, however, are insufficient to fully characterize the behavior of bodies because they do not distinguish between different types of materials.

Research in constitutive mechanics is concerned with the development of additional laws which serve to distinguish different types of material behavior. These laws, which are called constitutive laws or models, describe the macroscopic behavior resulting from the internal constitution of the material.

There are several approaches to the formulation of the constitutive models:

(i) Empirical models

These models employ mathematical expressions to fit experimental data. The approach is quite simple. However, it has a serious limitation in that the generalization of the model to allow for greater complexity in material behavior requires additional empiricism and the invocation of restrictive and/or invalid assumptions.

(ii) Phenomenological models

These models are generally based on the continuum theories of elasticity, plasticity, viscoelasticity, viscoplasticity, and continuum damage mechanics to formulate general functional constitutive equations. They seek to determine the limits imposed on the equations by the physical laws of thermodynamics, and are sometimes computationally tractable in engineering problem solving.
Generalized plasticity models have provided a convenient and computationally
elegant idealization for the nonlinear constitutive behavior of many materials even when
plasticity is not the underlying physical mechanism of deformation in the material, as in the
case of brittle materials.

Materials behave in such complex ways over the entire range of possible
temperatures and deformations that it is not feasible to develop a purely phenomenological
model to describe accurately a real material over the ranges of behaviors of interest. Consequently, such models are incapable of being used in boundary-value problems with
multiple mechanisms of deformation or where the mechanisms of deformation vary as a
function of space and time.

(iii) Micromechanical models

This type of model is based on the recognition that more general models can be
developed if the physical mechanisms operating at the scale of the material's
microstructures are taken into consideration.

The models provide detailed information concerning the constitutive behavior for
the specific mechanisms and are generally too complex mathematically and computationally
for use in engineering problem solving. However, these models are valuable in their ability
to guide, in a hierarchical and rigorous sense, the development of generalized constitutive
theories that are both physically-based and computationally tractable.

(iv) Physically-based but phenomenological constitutive models

Although considerable progress has been made in recent years, the
micromechanisms governing the deformation and failure of materials and their influence on
macroscopic behavior are not understood well enough to develop purely micromechanical
models of generalized constitutive behavior. However, it is often possible to capture the
overall characteristics of the micromechanisms through phenomenological models. This
approach may ultimately lead to the development of models which are not only physically based but also computationally tractable.

The main purpose of the present thesis is to develop a micromechanical model to describe the behavior and failure of brittle materials taking into account both the microstructural properties and the macroscopic phenomena where possible.

1.2 Micromechanical approach on the behavior of brittle materials

The overall mechanical response of brittle solids, such as rock, concrete and ice, is known to be characterized by the formation and propagation of internal microcracks; microcracking is the source of the inelastic behavior of brittle materials. Microscopic observations have shown that cracks may nucleate under axial compression at various microscopic inhomogeneities, such as grain boundary defects (ice) and the interface between dissimilar constituents (concrete). As the loading increases, the microcracks tend to grow toward the direction of the maximum compression, the compliance of the material increases, and the behavior becomes increasingly more nonlinear.

With no or relatively low confinement, there emerges a narrow region of high crack density which eventually becomes a fault plane and results in failure. At high confinement, the lateral force suppresses the growth of cracks and leads to either distributed microcracking or ductile flow produced by plastic deformation throughout the specimen (Horii and Nemat-Nasser, 1986).

Microscopic observations show that the frictional sliding of a pre-existing crack produces tension cracks at the crack tips at an angle close to 70° with respect to the flaw orientation. When the axial compression is accompanied by the lateral tension, the crack growth become unstable after a certain crack length is attained, resulting in axial splitting. On the other hand, with lateral compression the tension cracks stop growing after the crack length reaches a certain level.
Cracking also results in an increase in the compliance. In what follows, this effect is quantified.

Consider a elastic material damaged by distributed microcracks. The total strain is the sum of elastic strain and the strain due to damage:

\[ \varepsilon = \varepsilon_o + \varepsilon_d \]  
\[ \text{where} \]
\[ \varepsilon_o = S_o \sigma \]  
\[ \varepsilon_d = \frac{1}{A} \sum \frac{1}{2} \left( u n + n u \right) dl \]

In these expressions \( S_o \) is the undamaged or original compliance of the material, \( u \) is the crack opening displacement vector with unit normal vector \( n \), \( A \) is the unit area, and \( l \) is the length of the crack.

If the material is not homogeneous, as in the case of concrete, \( \varepsilon \) and \( \sigma \) are defined as the average strain and stress in the elastic matrix:

\[ \varepsilon = \frac{1}{A} \int \bar{\varepsilon} \ dA \]  
\[ \sigma = \frac{1}{A} \int \bar{\sigma} \ dA \]

where \( \bar{\sigma}, \bar{\varepsilon} \) represent the local stress and strain fields. From Eq. 1.1 to Eq. 1.3, the additional compliance \( H \) is defined by:

\[ H \sigma = \frac{1}{A} \sum \frac{1}{2} \left( u n + n u \right) dl \]
Finally the overall damaged compliance tensor $S$ is obtained by:

$$S = S_0 + H$$  \hspace{1cm} (1.7)

Under overall compressive forces, some pre-existing cracks may close, and this may introduce an anisotropic response to additional loadings. This anisotropy is load-dependent and is affected by the sequence of load applications. In plane strain, Hook's law is written as:

$$e_i = S_{ij} \tau_j, \quad i, j = 1, 2, 5$$  \hspace{1cm} (1.8)

For the isotropic and homogeneous case, the original compliance matrix $S_0$ becomes:

$$
\begin{bmatrix}
\frac{1-v^2}{E} & \frac{-v(1+v)}{E} & 0 \\
\frac{-v(1+v)}{E} & \frac{1-v^2}{E} & 0 \\
0 & 0 & \frac{2(1+v)}{E}
\end{bmatrix}
$$  \hspace{1cm} (1.9)

Crack closure under applied loads introduces an overall anisotropic response (Horii and Nemat-Nasser, 1983). In the self-consistent method, a single crack in an anisotropic elastic solid of compliance $S_{ij}$ is considered (Fig. 1.1). The displacement jump across a crack in an anisotropic, homogeneous, linearly elastic solid is given by Sih, Paris and Irwin (1965) as:

$$\left[ \nu' \right] = 2\sqrt{(c^2 - x^2)} S_{11} \left[ \left( \frac{\beta_1}{\alpha_1^2 + \beta_1^2} + \frac{\beta_2}{\alpha_2^2 + \beta_2^2} \right) \tau_{1}' + \frac{\alpha_1 \beta_2 + \alpha_2 \beta_1}{(\alpha_1^2 + \beta_1^2)(\alpha_2^2 + \beta_2^2)} \tau_{5}' \right]$$
\[
[u_2'] = 2\sqrt{\left(c^2 - x^2\right)}S_{22}'\left[\left(\alpha_1\beta_2 + \alpha_2\beta_1\right)\tau_1' + (\beta_1 + \beta_2)\tau_5'\right]
\] (1.10)

where \(c\) is the half length of the crack, and \(\lambda_1 = \alpha_1 \pm i\beta_1\) and \(\lambda_2 = \alpha_2 \pm i\beta_2\) are the roots of the characteristic equation

\[
S_{22}'\lambda^4 - 2S_{25}'\lambda^3 + \left(2S_{21}' + S_{55}'\right)\lambda^2 - 2S_{15}'\lambda + S_{11}' = 0
\] (1.11)

Note that in the self-consistent method, the overall compliance of the damaged material is used in the above equations.

The above equations apply to open cracks. For closed cracks:

if \(|\tau_5'| \leq |\mu \tau_1'|\) then \([u_1] = [u_2] = 0\)

if \(|\tau_5'| \geq |\mu \tau_1'|\) then \([u_1] = 0\)

\[
[u_2'] = 2\sqrt{\left(c^2 - x^2\right)}S_{22}'\left[\left(\alpha_1\beta_2 + \alpha_2\beta_1\right)\tau_1' + (\beta_1 + \beta_2)\left(\tau_5' + \mu \text{sgn}(\tau_5')\tau_1'\right)\right]
\] (1.12)

As a result, the final forms of the additional compliances are:

for an open crack:

\[
K_{11}' = \pi c^2\left(\frac{\beta_1}{\alpha_1^2 + \beta_1^2} + \frac{\beta_2}{\alpha_2^2 + \beta_2^2}\right)S_{11}'
\]

\[
K_{55}' = \pi c^2(\beta_1 + \beta_2)S_{22}'
\]

\[
K_{15}' = K_{51}' = \pi c^2(\alpha_1\beta_2 + \alpha_2\beta_1)S_{22}'
\] (1.13)
for a closed crack:

when \( |\tau_5^*| \leq |\mu \tau_1^*| \) then all \( K_{ij}^* = 0 \) and

when \( |\tau_5^*| \geq |\mu \tau_1^*| \) then

\[
K_{51}^* = \left( \alpha_1\beta_2 + \alpha_2\beta_1 \right) - \frac{[\alpha_1\beta_2 + \alpha_2\beta_1] - \mu \text{sgn}(\tau_5^*)(\beta_1 + \beta_2)\left[\frac{\beta_1(\alpha_2^2 + \beta_2^2) + \beta_2(\alpha_1^2 + \beta_1^2)}{\beta_1(\alpha_2^2 + \beta_2^2) + \beta_2(\alpha_1^2 + \beta_1^2)}\right]}{S_{22}^*}
\]

\[
K_{55}^* = \left( \beta_2 + \beta_1 \right) - \frac{[\alpha_1\beta_2 + \alpha_2\beta_1] - \mu \text{sgn}(\tau_5^*)(\beta_1 + \beta_2)\left[\frac{(\alpha_1\beta_2 + \alpha_2\beta_1)}{\beta_1(\alpha_2^2 + \beta_2^2) + \beta_2(\alpha_1^2 + \beta_1^2)}\right]}{S_{22}^*}
\]

(1.14)

otherwise \( K_{ij}^* = 0 \)

After obtaining the single crack contribution \( K \), the additional compliance \( H \) can be obtained by:

\[
H_{ij} = \frac{N}{\pi} \int_0^\pi K_{kl} T_{ki} T_{lj} d\theta
\]

(1.15)

where \( N \) is the number of cracks per unit area, \( T \) is the transformation matrix, and the crack is assumed to be randomly distributed in the material.

If the interaction effect is ignored, that is if the crack is imbedded in an unbounded solid whose instantaneous moduli coincide with those of the matrix material, the expressions for the displacement jumps and the single crack contribution to the additional compliance become (Horii and Nemat-Nasser, 1983):

for open cracks:
\[
[u_2'] = 4\sqrt{(c^2 - x^2)} \frac{1 - \nu^2}{E} \tau_5'
\]

\[
[u_1'] = 4\sqrt{(c^2 - x^2)} \frac{1 - \nu^2}{E} \tau_1'
\]  \hspace{1cm} (1.16)

\[
K_{11}' = K_{55}' = 2\pi c^2 \frac{1 - \nu^2}{E}, \text{ and other } K_{ij}' = 0
\]  \hspace{1cm} (1.17)

for the closed cracks with slip:

\[
[u_2'] = 4\sqrt{(c^2 - x^2)} \frac{1 - \nu^2}{E} (\tau_5' + \mu \text{sgn}(\tau_5') \tau_1'), [u_1'] = 0
\]  \hspace{1cm} (1.18)

\[
K_{55}' = 2\pi c^2 \frac{1 - \nu^2}{E}
\]

\[
K_{51}' = 2\pi c^2 \frac{1 - \nu^2}{E} \mu
\]  \hspace{1cm} (1.19)

1.3 Behavior of ice under loading

Ice covers more than 10% of the earth’s surface during the year, while nearly one-fifth of all land surface of the earth is underlain by perennially frozen earth of permafrost. The pace of development and construction, particularly in the polar and extreme subpolar zones, has become more rapid in recent years due to the needs for exploiting scarce natural resources.

The behavior of ice under load has led to great difficulties in quantifying the maximum loads it might exert on a structure. It is a creeping, ductile material at low strain rate loading, yet extremely brittle material at high stresses. Thus its behavior is dependent
on rate of deformation and deformation history. These mechanical properties have been extensively studied in the laboratory, leading to a secure understanding of the mechanical properties of ice. However, the strength of ice appears to be strongly scale-dependent: average stresses at failure measured under small-scale laboratory conditions tend to lie in the region of 10 MPa, while average stresses during full-scale interaction with a structure generally lie in the region of 1 MPa (Sanderson, 1988). This behavior is illustrated by the "pressure-area" curve (Fig. 1.2), which shows peak indentation pressure against gross contact area, as ice is indented by a wide variety of different sized indentors. This plot covers a vast range of scales from the smallest laboratory test on a scale of several millimeters to descriptions of behavior at the scale of many kilometers. It illustrates the problems involved in applying data acquired in a laboratory to interaction conditions which are different in scale by several orders of magnitude.

This research will focus on the prediction of the damage evolution due to microcracking and the failure stress of ice in specimen scale, as well as the microstructural investigation of the scale effects. The stress-strain relation of ice in the ductile-brittle transition will also be modeled. The results of this research are expected to provide a physically based model for the ice behavior under various loading conditions.

1.3.1 Problem Statement and Research Objectives

The problem of predicting the failure stress of ice is important to estimate ice loads on structures and the bearing capacity of ice. This problem is compounded by two phenomena: the scale or size effects governing the failure of ice during ice-structure interaction and the behavior of ice in the ductile-to-brittle transition range of strain rates. Although physically-based models have been proposed to characterize the strength of ice, they are generally of an empirical character and cannot be used for predictive purposes. These types of models are typically valid for uniaxial, constant strain-rate tests in
compression and are incapable of handling multiaxial stress states and change in strain rate or temperature.

Brittle materials have been shown to exhibit lower strengths with increase in size. The plots of failure stress versus contact area by Sanderson (1988) provide a clear picture of scale dependence in ice. There are two kinds of size related effects observed in ice, one involving the intrinsic strengths of ice as a material, the other involving failure mechanisms during ice-structure interaction, e.g., non-simultaneous failures. These effects are caused by: (i) the material scaling mechanisms which govern the variation of material behavior with scale; and (ii) the structural scaling mechanisms which govern the space-time variation of the deformation and failure mechanisms with scale in boundary-value problems. The material scaling mechanisms, which include both the Weibull-type weakest link phenomenon and fracture-related scaling mechanisms, are intimately tied to the actual microstructure of ice. The magnitude of the structural scaling mechanisms is controlled by parameters such as the loaded area, aspect ratio and the loading rate.

Statistical randomness in the physical and geometrical properties plays an important role in the deformation and failure of ice. Existing micromechanical models based on deterministic methods of analysis do not consider the statistical randomness of the microstructure. As a result, the observed scale effects and the large scatter in the experimental data cannot be explained.

The creep deformation of ice influences the nucleation of microcracks as well as the overall deformation of the ice matrix, especially when the strain rate is lower than that corresponding to the ductile-brittle transition. Cole (1988) suggests that the stress concentration associated with the pile-up of dislocations at grain boundary in ice reinforces those due to elastic anisotropy and lead to crack nucleation. Recent research has studied the crack nucleation mechanism in ice taking into account the stress concentration caused by both the crystal elastic anisotropy and dislocation pile-up mechanisms (Wu and Niu, 1994). However, a general constitutive model which can simulate not only the nucleation and the
growth of individual cracks but also the overall stress-strain response of the material with an evolving population of microcracks under multiaxial states, including macroscopic creep behavior, remains to be developed.

1.3.2 Brittle failure stress of ice

At strain rates lower than approximately $10^{-4}$ s$^{-1}$, ice is generally ductile and its stress-strain behavior is characterized by a peak between ascending and descending branch. When strain rates are increased more than approximately $10^{-3}$ s$^{-1}$, the material becomes brittle and the stress-strain curve has only an ascending branches (Schulson, 1990).

The behavior of ice in the brittle region is associated with the distributed cracking activity and the extension of localized macrocracks. In a uniaxial tension test the first crack to nucleate from the most favorably oriented precursor generally leads to sudden failure in the ductile to brittle transition and brittle regimes. In compression, sequential crack nucleation leads to a distribution of microcracks and progressive material damage.

In the ductile-brittle transition and brittle regime, the failure stress increases as the temperature and grain size decrease, and decreases as the strain rate increases. In tension, the nucleation of the first crack generally leads to splitting of the specimen. But in compression, two types of failure modes are reported: shear faulting, axial splitting and explosive failure. Shear faulting occurs when the nucleated cracks link together to form a localized shear band. Axial splitting occurs when appropriately located cracks propagate rapidly through the specimen (Schulson, 1990). The failure modes are known to be independent of the temperature and the grain size, but have a great relation with the end condition and the lateral confinement.

1.3.3 Behavior of ice under different scales
It is generally agreed that a brittle material displays a scale effect. Sanderson (1988) and Schulson and Zhang (1990) mention the mechanisms acting on the size effect of ice. The arguments concern the existence of flaws and tacitly make the assumption that flaws increase in size as sample size increases. Fig. 1.3 represents the two types of scale effects occurring in small scale specimen test. If the whole sample including the cracks is scaled up 10 times geometrically (Fig. 1.3(a)), then the enlarged sample contains flaws 10 times larger. In this case a fracture mechanics analysis will show that the fracture strength will decrease by a factor $10^{-0.5}$. Another class of scaling is shown schematically in Fig. 1.3(b). This contains the more realistic starting assumption that any material contains a statistical population of flaws of various sizes. On selecting a sample of larger size there is then a higher chance of it containing larger flaws. This Weibull type argument was intended principally for tensile fracture where the "weakest link" concept applies and a single controlling flaw is enough to lead to complete failure. Although this is not obviously true of compressive failure, especially in the case of shear faulting type failure where cracks join together to form a damaged band before a complete failure, the same argument can be applied in the failure by splitting where single crack propagates unstably throughout the specimen.

In real scale phenomenon, the leading edge of floating ice is generally irregular. Thus failure may occur non-simultaneously in discrete local zones. Although crushing may appear to be occurring over the full width $D$ of gross contact, at any specific time it is likely to be concentrated only in a few zones. A real-life example of the onset of such a process is shown in Fig. 1.3(c). As the zones fail in such a way that contact remains irregular throughout the impact process, they do not fail simultaneously. As a result, the average total load is reduced in a statistical fashion.

1.4 Research of concrete under short-term loading
Concrete is a composite material composed of coarse granular material embedded in a hard matrix of material that fills the space between the aggregate particles and glues them together. Due to its economical, casting and forming capabilities, concrete has been a popular structural material. However, concrete is a brittle material with very low tensile strength, which limits its use in certain applications.

It has been observed that the microstructure of concrete has a large number of cracks prior to any loading. These microcracks are formed by hydration, bleeding and segregation process. The nucleation, growth, interaction, and propagation of these microcracks leads to macroscopic failure of the material (Mindess, 1983).

The stress-strain relation of concrete deviates from linearity even at low loads and has a descending slope after maximum load, although the aggregate and the cement paste show brittle behavior. This difference between the deformation of concrete and the deformation of its constituents is mostly due to crack formation, even though part of the observed plasticity may be attributed to a viscous behavior of the hardened cement paste.

1.4.1 Fracture behavior of concrete under tension

It is observed that the stress-strain curve of concrete under uniaxial tension is linear up to 80% of the failure stress (Ziegeldorf, 1983). The deviation of the stress-strain diagram from linearity is linked to the enlargement of pre-existing bond cracks. At higher loads continuous cracks are formed from the individual bond cracks, and such continuous cracks normally lead to failure of the specimen. The tensile rupture of concrete is characterized by the formation of a surface which is perpendicular to the direction of tensile loading. For normal strength concrete the crack propagates in the matrix or along the interfaces. For high strength concrete the crack propagation through the aggregates may occur.
1.4.2 Fracture behavior of concrete under compression

It is reported that there are four stages in the deformation and failure of concrete (Mindess, 1983). The pre-existing defects in the aggregate-paste interfaces are stable up to 30-40% of the failure stress. At this stage, the bond cracks begin to nucleate along the interfaces, and their number increases as the external loading increases. Some of the bond cracks propagate into the paste to form mortar cracks. At 70-80% of the failure load the mortar cracks join with nearby bond cracks, forming continuous cracks. Sooner or later these continuous cracks reach a critical length and failure will occur. These processes are summarized in Fig. 1.4 with typical stress-strain curve.

Compared with the tensile test, the stress-strain curve may exhibit a pronounced descending branch. For higher strength concrete the stress-strain curve is steeper and linear up to a higher stress-strength ratio than in normal concrete because of a decrease in the amount and extent of bond cracking.

Under uniaxial compression failure occurs with vertical cracks, whereas with lateral confinement the failure is accompanied with inclined cracks. In high strength concrete the fracture surface is smoother and more vertical.

1.5 Research Approach and Methodology

The primary objectives of this doctoral thesis are to predict:
(i) failure stress of polycrystalline ice (Ch. 2)
(ii) effects of statistical randomness in micromechanical properties on the evolution of the elastic moduli and the failure stress of ice (Ch. 3)
(iii) specimen size effects on the brittle failure of ice (Ch. 4)
(iv) evolution of the elastic moduli of ice in the ductile-to-brittle transition (Ch. 5)
(v) damage evolution and tensile failure stress of plane concrete using the micromechanical model (Ch. 6)

1.5.1 Prediction of the failure stress of brittle ice

The failure strength of fresh water ice in high end of the ductile-to-brittle transition and brittle regions will be predicted by a micromechanical model. This model assumes the existence of starter cracks or precursors and takes into account the microstructural stress caused by the elastic anisotropy mechanism. The Coulombic frictional resistance between the crack faces is included in the computation of microcrack nucleation. Final failure is assumed to occur when one set of nucleated cracks satisfies the maximum principal tensile stress criterion and then propagates unstably. The effect of change in grain size, temperature and friction coefficient will be studied. The simulated results will be compared with the experimental data available in the literature. The possibility of crack linkage leading to formation of a shear band will not be considered in this research. As such, the results will provide an upper bound estimate of failure strength. This is conservative for ice loads prediction.

1.5.2 Statistical effects of microstructural properties on the failure stress of ice

The microstructural damage model from task 1 will be extended to consider the statistical effects caused by the randomness in microstructural parameters such as grain size and crystallographic orientation as well as microcrack length. Probability density functions representing the distribution of these parameters will be obtained using data from the published literature and from thin section photographs of ice. They will be used to predict the distribution of failure stress and the evolution of the compliance. A symmetric beta distribution will be used to represent the basal plane orientations of orthotropic S3 ice and
its initial compliance matrix. The evolution of the compliance with different orientation distributions of the basal plane will be studied. Other sources of statistical variation in microstructural properties, such as the spatial variation in the fracture toughness and the friction coefficient, will not be considered due to the paucity of experimental data.

1.5.3 Prediction of failure stress of finite-sized ice and the size effects

In this research the size effect in the strength of ice as a function of specimen scale will be investigated considering the interactions between the boundary and the cracks. The randomness in the microstructure of ice will be modeled using the graph model. The scale effects caused by the material scale mechanisms containing Weibull and fracture related scaling mechanisms will be studied with the computer generated microstructures. The analysis will take into account microstructural stresses and Coulombic friction at crack faces. The interaction between the nucleated cracks will be calculated using the superposition method and an approximation of certain unknown crack-line tractions by a series of base functions. The size effects will be studied by employing the boundary force method. In this method, concentrated forces and couples acting at various locations along an imaginary curve within an infinite medium are superposed to simulate the effect of an actual boundary. The failure stress will be predicted on the basis of the maximum principal stress criterion using various ice specimen sizes. The failure stress predicted with and without the boundary effect will then be compared.

1.5.4 Prediction of the ice behavior in the ductile-brittle transition domain

In this task the behavior of ice subjected to a strain rate in the ductile-brittle transition will be simulated. The mechanisms of dislocation pile-up and the elastic anisotropy will be considered in microcrack nucleation. The microcracks are assumed to
initiate at triple points and grow along the grain boundary until they are arrested at neighboring triple points. The grain boundary cracks will then sprout wings which extend into the neighboring crystals when the wedging forces resulting from sliding of the grain boundary cracks satisfy the maximum tensile principal stress fracture criterion. The evolution of the compliance will be computed considering the damage caused by the grain boundary cracks and wing cracks. The physically based phenomenological creep model developed by Shyam Sunder and Wu (1990) will be combined with the damage model to obtain a more general constitutive model for ice. It will be assumed that the damage process (i.e., evolution of elastic moduli) is not affected by the macroscopic creep deformation. LEFM will be applied to the crack nucleation and growth recognizing that the creep zone in front of the crack tip is small enough to apply the linear theory (Nanthikesan, 1992).

1.5.5 Prediction of the constitutive relation of concrete

In this task the constitutive relation of a plane concrete will be predicted using the micromechanical model developed for the previous tasks. The precursor is assumed to exist in the aggregate-hardened cement paste interface. The pre-existing defects are cause during hydration process, mainly by the non-homogeneity in elastic property of the constituent materials. When a fracture criterion is satisfied the pre-existing defects form bond cracks along the interfaces which have smallest fracture toughness. Once the bond cracks are formed they propagate into the mortar as the loading increases. Under tensile loading the wing crack is assumed to propagate unstably through the specimen as soon as it nucleates. Under compression, however, the wing crack grows gradually according to the loading, until it becomes unstable. In this study it is assumed that the unstable propagation of wing crack stops at the neighboring aggregates under compression, whereas it causes failure under tension. The overall compliance will be calculated from the damage due to
microcracks, and the predicted stress-strain curves will be compared with experimental data.
REFERENCES


Fig. 1.1 Local and global crack coordinate systems
Fig. 1.2 Pressure-area map of ice
Fig. 1.3 Scale effects occurring in specimen size brittle materials
Fig. 1.4 Damage process of concrete under uniaxial compression
CHAPTER II

PREDICTION OF BRITTLE FAILURE STRESS USING A MICROMECHANICAL MODEL

Abstract

In this study a micromechanical model is developed to predict the failure strength of polycrystalline ice in the brittle region. The model stipulates the existence of a starter crack or a precursor at the triple point of a grain boundary and of a microstructural stress field caused by an elastic anisotropy mechanism. The precursors nucleate into microcracks when the maximum principal stress criterion is satisfied. Final failure is considered to occur when the stress field at the tip of one or more of the nucleated cracks satisfies the same criterion. The surface energy based microstructural fracture toughness is used for predicting nucleation, whereas the macroscopic fracture toughness measures are used for failure. The effects of strain rate and temperature are considered by using appropriate friction coefficients and fracture toughnesses. The numerical predictions generally agree with the experimental data and can predict the increasing trend of the failure strength with increasing temperature and decreasing grain size and strain rate.

2.1 Introduction

The behavior of ice in the brittle and ductile-to-brittle transition ranges is of interest to engineers in predicting ice loads on structures and the bearing capacity of ice. At strain rates lower than approximately $10^{-4}$ s$^{-1}$, ice is generally ductile and its stress-strain behavior is characterized by a peak between ascending and descending branches. When the strain rate is greater than approximately $10^{-3}$ s$^{-1}$, the material becomes brittle and the stress-strain curve has only an ascending branch (Schulson, 1990).
Experimental results indicate that at the same strain rate in the transition regime, fine-grained specimens may exhibit more ductile behavior while coarse-grained material behaves in a more brittle manner (Cole, 1989). Thus, the increased cracking activity in the coarser-grained material causes the onset of brittle behavior at a lower strain rate than that found in fine-grained ice. The effect of grain size on the brittle failure stress is discussed in section 3.

In the ductile regime, the inelastic deformation of ice depends mainly on the dislocations on the basal plane and the associated strain hardening due to dislocations. The strain softening is associated with microstructural changes such as dynamic recrystallization and internal cracking (Cole, 1987).

The behavior of ice in the brittle region is characterized by the distributed cracking activity and the extension of localized macrocracks. Gold (1972) reported that the deterioration of the ice structure due to the crack activity causes the primary stage of creep to be transformed directly to the tertiary stage. Thus once cracking begins, the behavior of ice becomes brittle and this process dominates the deformation response of ice.

Experimental studies of cracking in ice have been undertaken by Gold (1972) and Sinha (1984) for columnar-grained S2 ice, and by Cole (1986, 1989) for polycrystalline ice. Cole (1989) identified four distinctive stages in the compressive failure process in the brittle regime: (1) elastic stage, (2) onset of crack nucleation and the increase of crack population, (3) end of nucleation and maintenance of stability, and (4) sudden and complete failure of the specimen. From these observation, it can be concluded that there is a distinct beginning and an end to the crack nucleation process prior to brittle compressive failure.

To explain the crack nucleation process, Sinha (1984) proposed the grain boundary sliding mechanism in which nucleation occurs at the grain triple points due to the stress concentration produced by the sliding along the grain boundaries. Kalifa et al. (1989) examined the dislocation pileup mechanism which is considered to cause a stress concentration as a result of plastic flow. From the observation that cracks form in a time
period too short for the pileup of dislocations to cause significantly large stress concentrations at the middle to high end of the ductile-to-brittle transition, Cole (1988) and Shyam Sunder and Wu (1990) have studied the elastic anisotropy mechanism as a main cause of crack nucleation. The dislocation pileup mechanism may continue to operate, but its effect becomes smaller as the loading rate increases.

In a uniaxial tension test, the first crack to nucleate from the most favorably oriented precursor generally leads to sudden failure in the ductile to brittle transition and brittle regimes. In compression, sequential crack nucleation leads to a distribution of microcracks and progressive material damage. In general there are two types of failure modes for ice under compressive loading: shear faulting and axial splitting. Shear faulting occurs when the nucleated cracks link together to form a localized shear band. Axial splitting occurs when appropriately located cracks propagate rapidly through the specimen. The failure modes are known to be independent of the temperature and the grain size, but dependent on the end conditions and lateral confinement. Schulson (1990) noted that shear faults occur when the specimens are compressed between bonded end caps, whereas splitting occurs when the specimens are compressed between brushes. In biaxial compression tests of columnar S2 ice, the direction of the ice columns and the magnitude of the confinement are important in determining the failure mode. Smith and Schulson (1992) find that under no across-column confinement and complete along-column confinement, failure occurs by splitting. Under a low degree of across-column confinement, failure occurs by shear faulting in the loading plane. At higher levels of across-column confinement, the specimen fails by out of surface fracture. Generally the failure strength corresponding to splitting is lower than the strength for a faulting type failure as might be expected. This is consistent with the observation that ice which fails by splitting has lower crack density, i.e., less energy from external loading is consumed by the crack nucleation process prior to final fracture. The same observation can be made in the higher strain rate tests which also show lower fracture stress.
There are two broad approaches for modeling damage accumulation and failure of ice: phenomenological and micromechanical. The phenomenological modeling approach based on continuum damage mechanics has been applied in the work of Sjöling (1987), Karr and Choi (1989), Santaoja (1989) and Mckenna et al. (1989), etc. In this approach, the damage is represented by a scalar, vector or tensorial variable with a characteristic evolution law. In the micromechanical modeling approach, physically definable material parameters are used to predict crack nucleation and damage evolution. Wu and Shyam Sunder (1992) combined the elastic anisotropy mechanism with the linear elastic fracture mechanics based maximum principal tensile stress criterion for crack nucleation, and formulated damage evolution in the framework of the self-consistent method. In their work the focus is on deformation and not the prediction of failure strength although they do assess the adequacy of the phenomenological critical crack density criterion to predict failure. Recently Wu and Niu (1993) predicted the compressive failure strength using a graph model to create possible microstructures for ice. Crack interaction is included in the computation of the stress field and the failure strength is obtained when the mode I stress intensity factor of a single crack reaches the macroscopic fracture toughness. They also concluded from their simulations that the crack density, representing the degree of global damage, may not be appropriate for predicting brittle failure which occurs in the weakest region of the specimen.

In this study the compressive failure strength at the high end of the ductile to brittle transition and the brittle regimes is predicted based on the micromechanical damage model of Wu and Shyam Sunder (1992). The model takes into account the microstructural stresses caused by the elastic anisotropy mechanism, as well as the Coulombic frictional resistance, in the process of crack nucleation from a precursor. The precursor, in turn, is a randomly oriented starter crack caused by the triple point singularity in the stress field due to the elastic anisotropy mechanism. A solid vapor surface energy based critical stress intensity governs the nucleation of microcracks while the direction of the nucleated cracks
is postulated to occur in a direction perpendicular to the local maximum tensile stress. Final failure is considered to occur when the most favorably located crack propagates in an unstable manner. The macroscopic polycrystal fracture toughness is used to predict the onset of failure. Whereas the unstable propagation of a single crack is assumed to produce instantaneous failure of the entire specimen, the present model is more appropriate for the splitting type failure frequently observed under uniaxial loading conditions. The numerical results are compared with experimental data obtained from both uniaxial and biaxial compression tests at various temperatures and strain rates.

2.2 Description of the micromechanical model

2.2.1 Microstructural stresses

Due to the elastic property mismatch between grains, the randomly oriented constituent crystals tend to deform in an incompatible manner. Since this incompatibility is not realized during continuum deformation, microstructural stresses are generated. The analysis of the microstructural stress is based on the first order approximation of the Eshelby (1957) procedure. A similar first-order approximation has been used by Evans (1984) to analyze the grain boundary residual stresses in isotropic ceramic polycrystals stemming from the thermal expansion anisotropy of individual crystals. Consider a precursor of length $2a$ with orientation $\beta$ and grains around it with various $c$-axis orientations as shown in Fig. 2.1. If the grains surrounding the precursor are separated from the polycrystal solid, the behavior of these grains can be defined in terms of the elastic stress-strain relations for single ice crystals, i.e.:

$$\varepsilon_g = S_g \sigma_a \quad (2.1)$$
where $\sigma_s$ is the applied stress, $\varepsilon_g$ and $S_g$ are the strain and the compliance of a single crystal, respectively. The remaining matrix has the elastic properties of the isotropic polycrystal solid, i.e.:

$$\varepsilon = S\sigma_s$$  \hspace{1cm} (2.2)

where $\varepsilon$ is the strain vector induced in the homogeneous matrix and $S$ is the compliance tensor of the polycrystal. When the solid is already damaged with cracks, the effective (damaged) compliance is used for $S$. Once the separated grains are fitted back to the polycrystal matrix, microstructural stress $\sigma_0$ is induced in the grain due to the misfit between the strain of the matrix and the strain of the crystal allowed to deform freely:

$$\sigma_0 = C_g(\varepsilon - \varepsilon_g)$$  \hspace{1cm} (3)

where $C_g$ is the stiffness matrix of a single crystal. In addition to the uniform microstructural stress produced by the first-order method, the microstress field in the vicinity of a grain boundary facet junction has a singularity proportional to $(1/r)^{\lambda}$ where $0<\lambda<1$ and $r$ is the radial distance from the grain boundary facet junction (Shyam Sunder and Wu, 1990). The stresses become singular as $r$ goes to the triple point. As the material cannot sustain such a singular stress field, precursors are formed at grain boundary junctions. In analogy with the work of Evans (1984) on ceramics, the precursor length $2a$ is taken to be ten percent of the grain size. Once a precursor is formed, it is assumed that the singularity is relieved, and the stress field ahead of the precursor tip is assumed to follow the classical LEFM inverse square-root singularity. Under uniaxial compression, the induced microstructural stresses due to elastic anisotropy in ice can be as large as 10 to 20 % of the applied stress, and they may be either tensile or compressive depending on the
crystallographic orientations of the grains. The nominal applied stress is enhanced as microcracks nucleate in the material. Consequently, the total stress results in:

\[
\sigma = \sigma_0(\zeta) + \sigma_a
\]  

(2.4)

where \(\sigma\) and \(\zeta\) denote the total stress and the basal plane orientation, respectively. The compliance matrix of a single ice crystal determined by Gammon et al. (1983) at the temperature \(T=\) \(-16^\circ\text{C}\) is given as follows.

\[
[S_8] = \begin{bmatrix}
1.0318 & -0.2316 & -0.4287 \\
0.8441 & -0.2316 & 0 \\
1.0318 & 3.3179 & 10^{-1}\text{GPa}^{-1}
\end{bmatrix}
\]  

(2.5)

where the plane of transverse isotropy is contained in the \(X_1\)-\(X_3\) plane, and the \(c\)-axis is in the \(X_2\) direction. The elastic constants of polycrystalline ice are determined by the distribution of the crystallographic orientation of each grain. The undamaged compliance matrix of isotropic granular ice at \(-16^\circ\text{C}\) are (Gammon et al. (1983)):

\[
[S] = \begin{bmatrix}
1.0716 & -0.3486 & -0.3486 \\
1.0716 & -0.3486 & 0 \\
1.0716 & 2.8401 & 2.8401 \\
sym & 2.8401 & 2.8401
\end{bmatrix}
\]  

(2.6)
Nanthikesan and Shyam Sunder (1993) theoretically computed the compliance matrix of the columnar grained transversely isotropic S2 ice at -16°C, which is:

\[
[S] = \begin{bmatrix} 1.0603 & -0.3540 & -0.3311 \\ 1.0603 & -0.3311 \\ 1.0318 & 3.1194 & \text{sym} & 3.1194 & 2.8286 \end{bmatrix} 10^{-1} \text{GPa}^{-1} \quad (2.7)
\]

where the plane of transverse isotropy is the \(X_1-X_2\) plane. The corresponding stiffness matrices can be obtained by inverting the compliance matrices.

The above 3-D matrices can be transformed into plane strain matrices using the relation given by Savin (1961). The transformed plain strain components of the compliance matrix of the single and polycrystalline ice become:

\[
[S_g] = \begin{bmatrix} 0.8537 & -0.3278 & 0 \\ 0.7921 & 0 & \text{sym} & 3.3179 \end{bmatrix} 10^{-1} \text{GPa}^{-1} \quad (2.8)
\]

\[
[S] = \begin{bmatrix} 0.9582 & -0.4620 & 0 \\ 0.9582 & 0 \text{sym} & 2.8401 \end{bmatrix} 10^{-1} \text{GPa}^{-1} \quad (2.9)
\]

And the plane strain compliance matrix of S2 ice is:

\[
[S] = \begin{bmatrix} 0.9541 & -0.4603 & 0 \\ 0.9541 & 0 \text{sym} & 2.8286 \end{bmatrix} 10^{-1} \text{GPa}^{-1} \quad (2.10)
\]
The elastic constants are known to be mildly affected by the temperature. Gammon et al. (1983) provided a correction formula for temperatures in the range of -5°C to -40°C and is given below:

\[ \Omega = \frac{1 - \omega T}{1 - \omega T_0} \tag{2.11} \]

where the parameter \( \omega \) has the value of \( 1.418 \times 10^{-3\,^\circ C^{-1}} \) and \( T_0 \) is the reference temperature in °C. The elastic constants at an arbitrary temperature \( T \) can be obtained by multiplying \( \Omega \) to the elastic constants given at the reference temperature.

2.2.2 Analysis of crack nucleation and propagation

If a local Cartesian coordinate \( X'_1-X'_2 \) is defined such that the \( X'_2 \) axis is parallel to the precursor, the stress field ahead of a precursor is characterized by the mode I and II stress intensity factors defined below:

\[ K_I = \sigma'_{11}\sqrt{\pi a} \quad K_{II} = \sigma'_{12}\sqrt{\pi a} \tag{2.12} \]

where \( a \) is the half precursor length which is equal to 10% of the grain size in this study. The component of the normal stress \( \sigma'_{11} \) and the effective shear stress \( \sigma'_{12} \) determined from the components in the unprimed frame can be represented as:

\[ \sigma'_{11} = \left( \sigma_{22} + \sigma_{11} \right) / 2 + \left[ \left( \sigma_{22} - \sigma_{11} \right) / 2 \right] \cos 2\beta - \sigma_{12} \sin 2\beta \]

\[ \sigma'_{12} = -\left[ \left( \sigma_{22} - \sigma_{11} \right) / 2 \right] \sin 2\beta - \sigma_{12} \cos 2\beta \pm \mu \sigma'_{11} \tag{2.13} \]
where \( \mu \) is the coefficient of friction and \( \mu \sigma'_{11} \) is the Coulombic frictional stress which opposes sliding when the normal stress is compressive. The effective shear stress \( \sigma'_{12} \) is set to zero when the applied stress is smaller than or equal to the frictional stress. If the normal stress is compressive, it is assumed that the crack is closed and consequently \( K_f = 0 \).

If we take \( r \) as the radial distance from the tip of the precursor and \( \theta \) as the angle measured anti-clock wise from a line extending along the precursor, the asymptotic distribution of the tangential and shear stress can be expressed as follows:

\[
\sigma_{\theta \theta} = \frac{1}{\sqrt{2\pi r}} \cos \frac{\theta}{2} \left[ K_I \cos^2 \frac{\theta}{2} - \frac{3}{2} K_{II} \sin \theta \right]
\]

\[
\sigma_{r \theta} = \frac{1}{2\sqrt{2\pi r}} \cos \frac{\theta}{2} \left[ K_I \sin \theta + K_{II} (3\cos \theta - 1) \right]
\]

(2.14)

The tangential stress \( \sigma_{\theta \theta} \) will be the principal stress when \( \sigma_{r \theta} \) is equal to zero, from which the two principal stresses can be obtained as:

\[
\sigma_{1,2} = \frac{1}{\sqrt{2\pi r}} \cos \frac{\theta_m}{2} \left[ K_I \cos^2 \frac{\theta_m}{2} - \frac{3}{2} K_{II} \sin \theta_m \right]
\]

(2.15)

where \( \theta_m \) is the angle that satisfies the relation \( \sigma_{r \theta} = 0 \), which is given by:

\[
\tan \frac{\theta_m}{2} = \frac{1}{4} \left[ \frac{K_I}{K_{II}} \pm \sqrt{\left( \frac{K_I}{K_{II}} \right)^2 + 8} \right]
\]

(2.16)

The precursor nucleates into a microcrack when the principal tensile stress given by Eq. 2.15 reaches the critical value for an equivalent mode I problem, \( k_{IC} / (2\pi r)^{1/2} \), and the nucleation criterion becomes:
\[ K_1 \cos^3 \frac{\theta_m}{2} - 3K_2 \cos^2 \frac{\theta_m}{2} \sin \frac{\theta_m}{2} = k_{IC} \]  

(2.17)

where the microstructural fracture toughness \( k_{IC} \) is determined from the effective surface energy \( \gamma \), the Young’s modulus \( E \), and the Poisson’s ratio \( \nu \) in the case of plane strain:

\[ k_{IC} = \sqrt{\frac{2E\gamma}{(1-\nu^2)}} \]  

(2.18)

At \( T=-16^\circ C \), the Young’s modulus and the Poisson’s ratio of the isotropic granular ice have the values of 9.332 GPa and 0.325, respectively. The corresponding values for S2 ice are 9.43 GPa and 0.334, respectively, in the plane of isotropy. The value of \( \gamma \) depends on whether the precursor extends along the grain boundary or into the crystal. In this study, the extension is assumed to be into the crystals and the solid vapor surface energy determined to be 0.109 Jm\(^{-2}\) by Ketcham and Hobbs (1969) is used. The solid vapor surface energy is known to be proportional to the elastic constants, but it is held constant in this analysis since the experimental data on its temperature dependency is not available. With the values given above, the plane strain value of the microscopic fracture toughness is \( k_{IC}=48 \) KPam\(^{1/2}\).

If the crack nucleation criterion is satisfied, the precursor grows as long as there is sufficient energy supply to overcome the resistance offered by obstacles such as grain boundary junctions or grains with unfavorable c-axis orientations. In the tensile experiments, strain rates greater than the ductile to brittle transition, the nucleation of the first crack determines the failure strength of ice since the applied tensile stress at nucleation is enough for propagation, while in compression the nucleated cracks stop growing when they confront obstacles. Once the nucleated cracks are arrested, they remain stable until a critical stress is reached. The mean crack length is proportional to the mean grain size, but the crack length is statistically distributed around the mean value. Cole (1986) constructed
a histogram of crack length distributions normalized by the mean grain size from experiments on laboratory grown fresh water granular ice. In this study the mean of the histogram, which is 50% of the grain size, is used for crack length and the kinked microcrack is simplified by a straight crack. Wu and Shyam Sunder (1992) has conducted a crack path analysis for the particular problem by stipulating that the precursor extends in a direction perpendicular to the maximum tangential stress. This criterion uses the complete stress criterion and is based on the assumption that the extension of the precursor does not significantly perturb the stress field. The schematic of the microcrack configuration used in this study is shown in Fig. 2.2.

The instability or failure condition is reached when the driving forces supplied by the applied stress field make the most favorably located microcrack propagate unstably. The resistance to this type of crack propagation is characterized in terms of the polycrystal or macroscopic fracture toughness. To formulate the crack propagation criterion the microcrack length $c$ and orientation $\chi$ are substituted in Eq. 2.12 and Eq. 2.13 instead of the precursor length $a$ and the precursor orientation $\beta$. The microscopic fracture toughness $k_{IC}$ is replaced by the macroscopic toughness measure $K_{IC}$ in Eq. 2.17. After such adjustments the fracture strength under biaxial compression can be obtained from Eq. 2.12, 2.13 and 2.17:

$$\sigma_{11}^f = \frac{K_{IC}}{\sqrt{\pi c}} \frac{1}{\left[ \frac{1 + \lambda}{2} - \frac{1 - \lambda}{2} \cos 2\chi \right] \cos^3 \frac{\theta_m}{2} - \frac{1}{3} \left[ \frac{1 - \lambda}{2} \sin 2\chi \pm \mu \right] \cos^2 \frac{\theta_m}{2} \sin \frac{\theta_m}{2}}$$

(2.19)

where $\sigma_{11}^f$ is the failure stress and $\lambda$ is the confinement ratio (i.e. ratio of lateral to axial stress).

The values of the macroscopic fracture toughness reported in Nixon and Schulson (1987) range from 70 to 140 KPa/m$^{1/2}$ for a temperature range from -50°C to -2°C, which are about two to three times higher than the microscopic fracture resistance. The
macroscopic fracture toughness is not significantly affected by changes in strain rate beyond the ductile-to-brittle transition regime.

The friction coefficient of ice, which provides a resistance to the sliding between crack surfaces and thus influences the crack nucleation and propagation process, is a function of the temperature and the sliding velocity of the precursor faces. Generally it increases as the temperature decreases and decreases as the strain rate increases (Schulson, 1990).

2.2.3 Crack density

When the precursor orientation $\beta$ and the basal plane orientation $\zeta$ are isotropically distributed from $-\pi/2$ to $\pi/2$, and the grain size is constant, the orientational damage $n(\beta)$ is the sum of the basal plane orientations satisfying Eq. 2.17 divided by the area of the $\beta$ - $\zeta$ space.

$$n(\beta) = \frac{1}{\pi^2} \int \Delta \zeta$$  \hspace{1cm} (2.20)

The overall damage, denoted by $D$, is the area fraction of the doublet $(\beta, \zeta)$ which satisfies the inequality in the two-dimensional $\beta$, $\zeta$ space:

$$D = \frac{\int_{-\pi/2}^{\pi/2} n(\beta) d\beta}{\pi}$$  \hspace{1cm} (2.21)

2.2.4 Elastic compliance of a damaged solid
The damaged compliance can be expressed as the sum of the undamaged compliance $S_{ij}$ and an additional contribution $H_{ij}$ due to the population of the nucleated microcracks:

$$\bar{S}_{ij} = S_{ij} + H_{ij}(\bar{S})$$  \hspace{1cm} (2.22)

If for a single crack $K'_{ij}$ denotes the contribution to the compliance as a function of the crack size and the crack opening displacement, then the additional compliance $H_{ij}$ can be computed as the product of the maximum number of precursors per unit area $M$ and the expected value of $K'_{ij}$ over the two random variables: crystal orientation and grain size.

When the crack length and the grain size are constant and the basal plane and the precursor orientations are uniformly distributed, the additional compliance becomes:

$$H_{ij} = \frac{M}{\pi^2} \int \int K'_iT_iT_j d\zeta d\beta$$  \hspace{1cm} (2.23)

where $T_{ij}$ denotes a transformation matrix. Using the formula for grain size proposed by Cole(1986) and taking the maximum number of precursors per grain to be 2 as shown by Wu and Shyam Sunder (1992) leads to $M=12/\pi d^2$. The components $K'_{ij}$ are given by Hori and Nemat-Nasser (1983). The limit of integration changes as the microcrack population increases. Generally, an iterative procedure is required to solve for the damaged compliance since it appears on both sides of the equation.

2.3 Discussion of model predictions

2.3.1 Parametric study
In this study, the effect of the material and geometric parameters, such as friction coefficient, fracture toughness and grain size, on the model prediction of the failure strength is demonstrated. The friction coefficient and fracture toughness are important factors in the numerical analysis because the effects of temperature and strain rate in the experimental data are introduced by appropriate choice of these parameters. Fig. 2.3 shows the failure strengths of isotropic granular ice at the temperature $T=-10^\circ C$ predicted by the numerical model with varying friction coefficient, macroscopic fracture toughness and grain size. In Fig. 2.3(a) friction coefficients of 0.3, 0.5 and 0.7 are used with the grain size varying from about 2 to 10 mm. The fracture toughness is set to 80 KPa m$^{1/2}$ in all the analysis. The results confirm that the failure strength increases as the friction coefficient increases. That is reasonable because the frictional resistance between crack surfaces reduces the effective shear stress on the crack. Similar results are obtained when the fracture toughness are changed from 70 to 90 KPa m$^{1/2}$ with a constant friction coefficient of 0.5 (see Fig. 2.3(b)). It also can be noted in both figures that the failure strength is proportional to the inverse of the square root of the grain size. The dependence of the failure stress on the lateral confinement is shown in Fig. 2.3(c) and, as expected, compressive confinement increases the failure stress and lateral tensile stress decreases it significantly.

2.3.2 Comparison with experimental data

Schulson (1989) presents experimental data on the brittle fracture stress of fresh water granular ice under uniaxial compression at temperatures from -10 to -50$^\circ C$ and strain rates of $10^{-3}$ and $10^{-1}$s$^{-1}$, for grain sizes varying from approximately 1 to 10 mm. Three sets of data from uniaxial compressive tests are taken and compared with the numerical predictions. The test conditions in each sets of experiments are: (i) $T=-10^\circ C$, $\dot{\varepsilon}=10^{-3}$s$^{-1}$, (ii) $T=-50^\circ C$, $\dot{\varepsilon}=10^{-3}$s$^{-1}$, and (iii) $T=-10^\circ C$, $\dot{\varepsilon}=10^{-1}$s$^{-1}$. These conditions are considered in
the numerical model by selecting proper values for the friction coefficient and the macroscopic fracture toughness from experimental data: (i) $\mu=0.5$, $K_{IC}=80KPa m^{0.5}$ (ii) $\mu=0.85$, $K_{IC}=130$ (iii) $\mu=0.15$, $K_{IC}=80$. A fourth experimental data set for fracture strength in uniaxial tension at $T=-10^\circ C$ and $\dot{\varepsilon}=10^{-3}s^{-1}$ is taken from Schulson (1989). The data are compared with the model prediction of the nucleation stress evaluated with the condition $\mu=0$, $k_{IC}=48KPa m^{0.5}$. Fig. 2.4(a) and (b) compare the test data and the numerical predictions from the model analysis. In Figure 2.4(b) the nucleation of the first crack is taken to be the tensile failure and the results are compared with the experimental data obtained at $T=-10^\circ C$ at $\dot{\varepsilon}=10^{-3}s^{-1}$ (Schulson, 1989). The numerical results for the tensile failure stress slightly overestimate the experimental data and form an upper bound of the experimental data. According to the figures, the failure strength increases as much as 100% as the temperature changes from $-10^\circ C$ to $-50^\circ C$ at the strain rate of $10^{-3}s^{-1}$. This phenomenon may be explained by the observation that both the fracture toughness and the friction coefficient increases as the temperature decreases. The experimentally measured macroscopic fracture toughness does not change with the strain rate over the range considered in the experiments. Fig. 2.4(a) and 2.4(b) also show that as the strain rate increase the failure strength decreases, which may be partly due to the decrease in the friction coefficient with increasing strain rate.

It is evident in Figure 4 that the failure strength increases as the grain size decreases at strain rates above the transition point. This is to be expected because coarse grained ice is more susceptible to cracking activity. In addition, the fracture toughness increases slightly with decreasing grain size as reported in Nixon and Schulson (1987). The increase in fracture toughness provides greater resistance to the propagation of the microcracks and this increases the stress at failure. The data in case (iii) ($T=-10^\circ C$, $\dot{\varepsilon}=10^{-1}s^{-1}$) deviate from the linear line as the grain size decreases. In fine grained ice, where the ice may remain in the ductile region, plastic flow is present in the deformation process and serves to reduce the failure stress (Cole, 1987).
The axial strain ($\varepsilon_{11}$) and lateral strain ($\varepsilon_{22}$) at failure predicted by the numerical model are plotted in Fig. 2.5 as a function of grain size. The results show that maximum strain increases as the grain size decreases and decreases as the strain rate increases as observed by Cole (1987). The predicted maximum strains vary from about 0.04 to 0.12% at the strain rate of $10^{-3}$ s$^{-1}$ and from about 0.02 to 0.1% at $10^{-1}$ s$^{-1}$. Those results agree with the experiments by Schulson (1989) who states that failure occurs after an axial strain of about $10^{-3}$ is reached, but are slightly smaller than the experimental data of Cole (1987) conducted at $T=-5^\circ$C, which vary from 0.15 to 0.25% and 0.05 to 0.15% at corresponding strain rates and grain sizes. The creep strain may have worked to produce higher strain in the experimental results. At higher strain rates where the effects of creep is relatively small, the predicted maximum strain is closer to the experimental data.

Fig. 2.6 compares the predicted nucleation stress with the failure strength. The failure strength is about two to three times higher than the nucleation stress, which matches with the observation that brittle compressive fracture does not occur upon the formation of the first crack but after the ice is damaged by the accumulation of microcracks (Schulson, 1990).

The model prediction of the compliance and the overall damage at failure are plotted in Fig. 2.7 and Fig. 2.8, respectively. Interestingly, the compliance and the damage at failure are independent of the grain size, but are dependent on the strain rate and the temperature. According to the predictions, the compliance and the overall damage become larger when the temperature and the strain rate go up. These are caused by the fact that the friction coefficient between the crack faces becomes smaller as the strain rate and the temperature increase (Schulson, 1990), making the crack nucleate more easily.

Smith and Schulson (1993) investigated the brittle compressive failure of fresh water columnar S2 ice under biaxial loading at a strain rate of $10^{-2}$s$^{-1}$ and temperatures of $-10^\circ$ and $-40^\circ$C. Tests were performed through proportional loading over the range of $0<\lambda<1$ where $\lambda$ is the ratio of the minor to major compressive stress. Under the across
column confinement, the experimental failure stress increases rapidly with increasing confinement when $0 < \lambda < \lambda_t$ and then decreases as $\lambda$ increases further. $\lambda_t$ is the transition confinement ratio at which the failure stress begins to decrease, and is determined as 0.2 at -10°C and 0.1 at -40°C. The failure mode identified are: (i) splitting along the columns at zero confinement, (ii) shear faulting in the loading plane when $\lambda$ is less than $\lambda_t$, (iii) shear faulting out of the loading plane when $\lambda$ becomes greater than $\lambda_t$.

In this study with the plane strain approximation, only the in-plain failure strength is predicted. Using a friction coefficient of 0.4 and macroscopic fracture toughness of 80 kPa m$^{1/2}$ to model the data obtained at a temperature of -10°C and 110 kPa m$^{1/2}$ for the data at -40°C, the numerical predictions form an upper bound of the experimental data at a given confinement ratio as shown in Fig. 2.9.

2.4 Conclusions

In this study a micromechanical model is developed to predict the failure strength of fresh water ice by the micromechanical model based on the elastic anisotropy mechanism and linear elastic fracture mechanics. A precursor or a small starter crack is assumed to exist as a result of the singularity at the triple point, and is made to nucleate into a microcrack when the maximum principal stress criterion, a form of mixed mode linear elastic fracture criterion, is satisfied. The model assumes that the most favorably oriented microcrack propagates unstably once the same failure criterion is satisfied and that this propagation directly leads to failure. A surface energy based micromechanical fracture toughness is used to determine the nuclelation of microcracks from precursors, and macro fracture toughness measures are used to predict failure. The model predictions are made with grain sizes ranging from about 1 to 10 mm, strain rates from $10^{-3}$ to $10^{-1}$ s$^{-1}$, and temperatures from -10°C to -50°C. It is worth mentioning that by ignoring crack
interactions the model provides upper-bound prediction of the failure strength, which is conservative for engineering design of offshore structure to resist ice loads.

The conclusions of this paper are as followings:

1. The model predictions of the fracture strength of fresh water ice are in good agreement with the experimental data.

2. The model predictions confirm experimental trends that the failure strength is inversely proportional to the square root of the grain size and that it increases as the temperature and the strain rate decrease.

3. The model predictions conform with the experimental observation that the failure strength is two to three times higher than the crack nucleation stress.

4. The existence of any lateral confinement deters the failure.

5. The strain at failure obtained from the model prediction forms the lower bound of the experimental data.

7. The compliance and the overall damage at failure predicted by the model are insensitive of the grain size, but are dependent on temperature and strain rate. They become greater as the strain rate and the temperature go up.
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Fig. 2.1 Orientations of the precursor and the basal planes
Fig. 2.2 Approximation of the microcrack orientation
Fig. 2.3(a) Effect of the friction coefficient on the failure stress

Fig. 2.3(b) Effect of the fracture toughness on the failure stress
Fig. 2.3(c) Effect of the confinement on the failure stress
Fig. 2.4(a) Comparison of model predictions for the failure stress of ice with the experimental data of Schulson (1989), (i) data from uniaxial compression tests (T=−10°C, \( \dot{\varepsilon} = 10^{-3}s^{-1} \)), (ii) model predictions with \( \mu = 0.5, K_{IC} = 80 \text{ KPa}m^{0.5} \), (iii) data from uniaxial tensile tests (T=−10°C, \( \dot{\varepsilon} = 10^{-3}s^{-1} \)), (iv) model predictions with \( \mu = 0, K_{IC} = 48 \text{ KPa}m^{0.5} \).
Fig. 2.4(b) Comparison of model predictions for the failure stress with the experimental data of Schulson (1989), (i) data from uniaxial compression tests ($T=-10^\circ C$, $\dot{\varepsilon}=10^{-1}s^{-1}$), (ii) model predictions with $\mu=0.15$, $K_{IC}=80$ KPa$m^{0.5}$, (iii) data from uniaxial compression tests ($T=-50^\circ C$, $\dot{\varepsilon}=10^{-3}s^{-1}$), (iv) model predictions with $\mu=0.9$, $K_{IC}=130$ KPa$m^{0.5}$
Fig. 2.5(a) Model predictions of maximum axial and lateral strain at failure

Fig. 2.5(b) Model predictions of maximum volumetric strain at failure
Fig. 2.6 Nucleation stress vs. failure stress, (i) model predictions of failure stress with $\mu=0.5$ and $K_{IC}=80$ KPa$m^{0.5}$. (ii) model predictions of nucleation stress with $\mu=0.5$ and $K_{IC}=48$ KPa$m^{0.5}$.
Fig. 2.7(a) Lateral compliance at failure

Fig. 2.7(b) Shear compliance at failure
Fig. 2.8 Overall damage at failure
Fig. 2.9 Comparison of the simulated biaxial failure stresses with the experimental data by Smith and Schulson (1993), (i) data from biaxial compression tests (T=-10°C, $\dot{\varepsilon}=10^{-2}$s$^{-1}$), (ii) model predictions with $\mu=0.4$, $K_{IC}=80$ KPa$m^{0.5}$, (iii) data from biaxial compression tests (T=-40°C, $\dot{\varepsilon}=10^{-2}$s$^{-1}$), (iv) model predictions with $\mu=0.8$, $K_{IC}=110$ KPa$m^{0.5}$
CHAPTER III

STATISTICAL EFFECTS ON THE EVOLUTION OF COMPLIANCE AND FRACTURE STRESS

Abstract

The large scatter in the experimental data of a brittle polycrystalline material, such as ice, is partly due to the difference in the microstructure. A micromechanical damage model of Kim et. al (1995) is used to investigate the statistical effects caused by the randomness in the microstructural properties such as: microcrack length, grain size and crystallographic orientation. Probability density functions are constructed from experimental data to represent the distribution of parameters, and are used to predict the evolution of the compliance. A probability theory is used to formulate the probabilistic distribution of the failure stress and the compliance caused by the distribution of the underlying microstructural parameters. The 10 to 90th percentiles of the failure stress obtained from the model analysis reasonably match with the scatter in the experimental data.

3.1 Introduction

According to the experiments on ice, the deformation behavior of ice in the ductile-brittle transition and brittle region is dominated by the nucleation and propagation of microcracks.

Based on physical processes of ice, Wu and Shyam Sunder (1992) proposed a microstructural model of damage evolution based on the elastic anisotropy mechanism in ice. They stipulated the existence of a starter crack or a precursor in grain boundary triple junctions and included the influence of the microstructural stress which helps the precursor
propagate into a microcrack when a fracture criterion is satisfied. The microstructural model is combined with macroscopic constitutive law by Horii and Nemat-Nasser (1983) to make the evolution equation of compliance due to growing number of microcracks. In their computation, the grain size and the microcrack length are held fixed, and the basal plane and the precursor orientation are assumed to be uniformly distributed.

In reality, however, there are many sources of statistical variation in the microstructure of ice. From experiments on compressive fracture of ice, Shulson (1990) suggests that the large scatter in the brittle compressive fracture stress, compared with the smaller degree of scatter in the ductile peak compressive strength, is more a characteristic of brittle behavior of ice than a manifestation of experimental error. The large distribution in micromechanical parameters makes it necessary to use the statistical expression in the quantitative representation of the numerical results.

Considering the fact that the grain size is not constant even in the ice made under laboratory controlled condition, Wu and Shyam Sunder (1992) included the probability density function (PDF) of crack length and grain size in their damage model to show the effect of variation of the parameters on the evolution of compliance. They used two parameter gamma distribution to model the distribution of grain size. The distribution of crack length is determined from the linear relation between grain size and crack length proposed by Cole (1986). The probability density functions of the grain size satisfy the mathematical requirements they need, but they are not based on experimental data. Furthermore, as the change in compliance is shown after averaging process, the amount of scatter of the resultant compliance caused by the variation of the input parameters is still unknown.

In this study, the PDF of the grain size variation is obtained based on the histogram constructed from an ice thin section photograph. The PDF of crack length is obtained from the histogram of the crack length normalized by the mean grain size constructed by Cole (1986) from experiments of about 40 ice specimens. These density functions are used in
the formulation for the evolution and variation of the compliance. Also the effect of the non-uniform distribution of the basal plane orientation on the evolution of compliance is investigated. It is interesting to note that the formulation of the evolution equation considering non-uniform distribution of the basal plane leads to the damage modeling of the S3 ice which is a special type of columnar grained ice.

3.2 Description of the micromechanical model

The proposed model incorporates the microstructural stress caused by the elastic anisotropy as well as the Coulombic friction between crack faces in the analysis. A microcrack is assumed to nucleate from a precursor which forms at the triple junction of grain boundaries due to the elastic property mismatch between the grains. As the loading increases more and more precursors nucleate into microcracks, resulting in accumulation of damage. The macroscopic damage evolution is computed by the method of Horii and Nemat-Nasser (1983) which analyzes the contribution of individual cracks in an effective medium. The final failure is defined when one of the most favorably oriented microcracks propagates unstably. The maximum principal tensile stress criterion of Erdogan and Sih (1963) is used for both nucleation and propagation of the microcracks.

3.2.1 Microstructural stresses and the precursor formation

The microstructural stresses are made up of a uniform component and a non-uniform component with singularity (Evans, 1978). The uniform component \( \sigma_0 \) results from the mismatch in property between the two adjacent grains adjoining the grain boundary, and is the first order approximation of the total stress computed by the procedure developed by Eshelby (1957), which is:
\[
\sigma_o = \frac{1}{2} \left\{ \left[ C_8(z_1) + C_8(z_2) \right] S - 2I \right\} \sigma_a
\]  

(3.1)

where \(C_8\) is the stiffness matrix of single ice crystals in the global reference frame. The letter \(z_1\) and \(z_2\) denote the basal plane orientations of the adjoining grains shown in Fig.3.1. The matrix \(S\) represents the compliance matrix of the polycrystal, and \(\sigma_a\) is the applied remote stress field. The total stress is the summation of the remote stress and the microstructural stress. The compliance matrix of a single ice crystal determined by Gammon et al. (1983) at temperature \(T=\text{-}16^\circ\text{C}\) are given as follows.

\[
\left[ S_8 \right] = \begin{bmatrix}
1.0318 & -0.2316 & -0.4287 \\
0.8441 & -0.2316 & 0 \\
1.0318 & 3.3179 & 10^{-1} \text{GPa}^{-1}
\end{bmatrix}
\]

(3.2)

where the plane of the transverse isotropy is contained in the \(X_1\)-\(X_3\) plane, and the \(c\)-axis is in the \(X_2\) direction. The stiffness matrix of a single ice crystal can be obtained by inverting the compliance matrix. The elastic constants of polycrystalline ice are determined by the distribution of the crystallographic orientation of each grain. The undamaged compliance matrix of isotropic granular ice at \(\text{-}16^\circ\text{C}\) are (Gammon et al. (1983)):

\[
[S] = \begin{bmatrix}
1.0716 & -0.3486 & -0.3486 \\
1.0716 & -0.3486 & 0 \\
1.0716 & 2.8401 & \text{\text{sym}}
\end{bmatrix}
\]

\(10^{-1} \text{GPa}^{-1}\)  

(3.3)
3.2.2 Nucleation of microcracks

The formulation of microcracking procedure takes into account the combined stress field generated by both the applied and the microstructural stress. Consider the precursor which is oriented at an angle \( \beta \) with the \( X_1 \) axis and is subjected to the total remote normal stress \( \sigma'_{11} \) and shear stress \( \sigma'_{12} \) defined in a local coordinate \( X'_1-X'_2 \):

\[
\sigma'_{11} = \left( \sigma_{22} + \sigma_{11} \right)/2 + \left[ (\sigma_{22} - \sigma_{11})/2 \right] \cos 2\beta - \sigma_{12} \sin 2\beta
\]

\[
\sigma'_{12} = -\left[ (\sigma_{22} - \sigma_{11})/2 \right] \sin 2\beta - \sigma_{12} \cos 2\beta \pm \mu \sigma'_{11}
\]  

(3.4)

where \( \mu \) is the coefficient of friction and \( \mu \sigma'_{11} \) is the Coulombic frictional stress which oppose sliding when the normal stress is compressive. The effective shear stress \( \sigma'_{12} \) is set to zero when the applied stress is smaller than or equal to the frictional stress. The mode I and II stress intensity factors become:

\[
K_I = \sigma'_{11} \sqrt{\pi a}
\]

\[
K_{II} = \sigma'_{12} \sqrt{\pi a}
\]  

(3.5)

where \( a \) is the half precursor length. If the normal stress is compressive, it is assumed that the crack is closed and consequently \( K_I = 0 \). The asymptotic distribution of the tangential and shear stresses can be expressed as follows:

\[
\sigma_{\theta\theta} = \frac{1}{\sqrt{2\pi r}} \cos \theta \left[ K_I \cos^2 \frac{\theta}{2} - \frac{3}{2} K_{II} \sin \theta \right]
\]
\[ \sigma_{r\theta} = \frac{1}{2\sqrt{2\pi r}} \cos \theta \left[ K_1 \sin \theta + K_{II} (\cos \theta - 1) \right] \] (3.6)

where \( r \) is the radial distance from the tip of the precursor and \( \theta \) is the angle measured anti-clockwise from a line extending along the precursor in the solid.

The maximum principal tensile stress criterion is used as a crack nucleation criterion, which stipulates that a precursor extends into a microcrack when the following expression reaches the microscopic fracture fracture toughness \( k_{IC} \):

\[ K_1 \cos^3 \frac{\theta_m}{2} - 3K_{II} \cos^2 \frac{\theta_m}{2} \sin \frac{\theta_m}{2} = k_{IC} \] (3.7)

where \( \theta_m \) is obtained by setting the \( \sigma_{r\theta} \) in Eq.3.6 equal to zero, which is given by:

\[ \tan \frac{\theta_m}{2} = \frac{1}{4} \left[ \frac{K_1}{K_{II}} \pm \sqrt{\left( \frac{K_1}{K_{II}} \right)^2 + 8} \right] \] (3.8)

The microstructural fracture toughness \( k_{IC} \) is determined from the effective surface energy \( \gamma \), the Young's modulus \( E \), and the Poisson's ratio \( \nu \):

\[ k_{IC} = \sqrt{2E\gamma} \quad \text{plane stress} \]

\[ k_{IC} = \frac{2E\gamma}{\sqrt{1 - \nu^2}} \quad \text{plane strain} \] (3.9)

The value of \( \gamma \) depends on whether the precursor extends along the grain boundary or into the crystal. In this study the extension into the crystals is assumed and the solid vapor surface energy determined to be 0.109 Jm\(^{-2}\) by Ketcham and Hobbs (1969) is used.
Eq. 3.8 yields two critical initial angles and the angle that yields the most positive value in Eq. 3.7 is chosen and compared with $k_{IC}$. Eq. 3.7 represents the kinetic law of microcrack evolution, and as the applied stress is increased nucleation maps can be plotted in the $\beta - \zeta$ space. The precursor extends in a direction perpendicular to the maximum tangential stress and the crack path analysis requires an evaluation of the stress field around a precursor at each nucleation site ($\beta, \zeta, d$) where the microcracking criterion is satisfied.

The resulting crack profiles are generally curved and approximated by straight lines of orientation $\chi$ (see Wu and Shyam Sunder (1992)).

### 3.2.3 Elastic compliance of a damaged solid

The damaged compliance $S$ can be computed using the theory developed by Horii and Nemat Nasser (1983). It can be divided into the original compliance $S_0$ and the additional compliance $H$ generated from the nucleation of the microcracks:

$$ S = S_0 + H $$  \hspace{1cm} (3.10)

The plane stress representation of the undamaged compliance is given by the following matrix:

$$ [S] = \frac{1}{E} \begin{bmatrix} 1 & -\nu & 0 \\ -\nu & 1 & 0 \\ 0 & 0 & 2(1+\nu) \end{bmatrix} \hspace{1cm} (3.11) $$

where $E$ and $\nu$ denote the Young's modulus and the Poisson's ratio, respectively. The additional compliance $H$ can be expressed as following when the crack length and the
grain size are constant, and the orientations of the precursor and the basal plane are uniformly distributed from 0 to $\pi$:

$$H_{ij} = \frac{M}{\pi^2} \int K'_{ij} T_j T_i \ d\zeta \ d\beta$$  \hspace{1cm} (3.12)

where $M = 12/\pi d^2$ represents the maximum number of precursors per unit area in the given stress assuming that there are maximum number of 2 precursors per grain and the number of microcracks per grain is $6/\pi d^2$ (Cole, 1986), and $K'$ is the single crack contribution to the additional compliance given in Horii and Nemat-Nasser (1983).

3.2.4 Fracture stress

Under the strain rates greater than the ductile to brittle transition, the strength of ice depends on the nucleation and/or propagation of the microcracks. In tension the first crack nucleation from a favorably oriented precursor generally leads to a sudden failure. But in compression the sequential nucleation leads to distributed cracking and progressive material damage. When ice is loaded with uniaxial compression it fails by an axial splitting, whereas under biaxial compression the nucleated cracks link together to form a localized shear band. In this study the maximum principal tensile stress criterion is used to predict the brittle failure of ice.

Once a microcrack nucleates from a precursor, it remains stable until a further loading causes the microcrack to propagate. To obtain the fracture stress the crack length $c$ and the orientation $\chi$ are used in Eq. 3.4 and 3.5 instead of the precursor length $a$ and orientation $\beta$. The microscopic fracture toughness is replaced by the macroscopic fracture toughness measured by Nixon and Shulson (1987) in Eq. 3.7. It ranges from 0.08 to 0.13 MPam$^{0.5}$ as the temperature changes from -2$^\circ$ to -50$^\circ$C. The macroscopic fracture toughness is independent of the strain rate, and is 2-3 times higher than the microscopic
toughness measure. When Eq. 3.7 is satisfied after the above adjustments, the total stress at failure $\sigma_f$ becomes:

$$\sigma_{11}^f = \frac{K_{IC}}{\sqrt{\pi} \epsilon} \left[ \frac{1 + \lambda}{2} - \frac{1 - \lambda}{2} \cos 2\chi \right] \cos^3 \frac{\theta_m}{2} - 3 \left[ \frac{1 - \lambda}{2} \sin 2\chi \pm \mu \right] \cos^2 \frac{\theta_m}{2} \sin \frac{\theta_m}{2} \right]^{(3.13)}$$

where $K_{IC}$ is the macroscopic fracture toughness and $\lambda$ is the confinement ratio.

The prediction of the fracture stress through Eq. 17 is found to be consistent with the experimental results (Kim et. al., 1995).

3.3 Effect of the statistical distribution of microstructures

3.3.1 Variation of microcrack length

In this section, the scatter of the failure stress and the compliance is predicted based on the scatter of the microstructural parameters. For that purpose, the PDF of the crack length and the grain size are obtained from experimental data, and they are used to get the probability density function of the failure stress and the additional compliance through a simple probability theory.

The size of a crack at a given temperature depends on the applied stress and the microstructural characteristics of the polycrystalline aggregate, such as the orientation, shape and size of the grains. Under certain conditions, these cracks propagate only a short distance before coming to rest within the material. Given sufficiently high stress levels, the cracks can propagate through the material to cause brittle fracture. In compression, when cracks do not propagate, they are responsible for the gradual weakening of the structure as straining proceeds.
A significant relationship between the grain size and the internal cracking of polycrystalline ice has been reported (Cole, 1986). Cole showed the average crack length plotted against the average grain diameter, along with the least-squares best fit curve for all data points. He also showed a histogram of all the crack length data normalized by the mean grain size, which is reproduced in Fig. 3.2. The distribution of the merged normalized data retains essentially the same shape as the raw crack length data of the individual specimens. Given the observation, it appears likely that a generalized distribution in terms of normalized crack length may be used to estimate the actual crack length distribution for any given mean grain size without any computational effort.

The PDF of the normalized crack length $x$ can be obtained by fitting the given histogram to one of the existing density functions. Two parameter Weibull distribution is applied first for that purpose because it has advantage in fitting the numerical data. If $\alpha$ and $\beta$ are taken as its parameters, its functional form is given by:

$$f_X(x) = \alpha \beta^{-\alpha} x^{\alpha-1} \exp(-\beta^{-\alpha} x^\alpha) \quad x > 0, \; \alpha > 0, \; \beta > 0$$

(3.14)

where $x = \frac{2c}{d}$ in this case. Weibull distribution has an explicit expression for the cumulative distribution function (CDF), which is:

$$F_X(x) = 1 - \exp(-\beta^{-\alpha} x^\alpha)$$

(3.15)

Estimation of the parameters $\alpha$ and $\beta$ of the Weibull distribution is somewhat difficult to do. There exist analytical methods for estimating parameters, but a more rapid and commonly used method, based on a graphical technique, is used here. This method is based on the fact that the CDF of the Weibull distribution can be transformed into a linear function of $\log x$ by means of a double-logarithmic transformation:
\[
\log \left[ \ln \frac{1}{1 - F_X(x)} \right] = \alpha \log x - \alpha \log \beta
\] (3.16)

and it can be seen that the right-hand side is linear in \( \log x \). If given data points fall reasonably close to a straight line after this transformation, it can be assumed that the underlying distribution follows the Weibull type distribution. The parameters of this distribution can be estimated by applying the linear regression method to fit a straight line to the transformed data. Fig. 3.2(b) shows the probability density function of the normalized crack length \( x \) obtained by the above procedure. Once the PDF of the normalized crack length is found, the PDF of the crack length with constant grain size can be obtained through following relation:

\[
f_C(c) = \frac{dx}{dc} f_X(x) = \alpha \left( \frac{\beta d}{2} \right)^{-\alpha} c^{\alpha-1} \exp \left[ - \left( \frac{\beta d}{2} \right)^{-\alpha} c^\alpha \right]
\] (3.17)

which is also a Weibull distribution with parameter \( \alpha \) and \( \beta d/2 \).

The Weibull distribution is quite useful in most cases. But for the distribution of the failure strength due to the grain size distribution the log-normal distribution turns out to provide a better fit for the numerical results. The functional form of the log-normal distribution is:

\[
f_X(x) = \frac{1}{\sqrt{2\pi x^\beta}} \exp \left[ - \frac{(\ln x - \alpha)^2}{2\beta^2} \right]
\] (3.18)

where \( \alpha \) and \( \beta \) are the parameters of the function. The probability that a random variable having the log-normal distribution will take on a value between \( a \) and \( b \) (\( 0 < a < b \)) can be obtained by:
\[ f_{a}^{b} \frac{1}{\sqrt{2\pi}\beta} x^{-1} \exp \left[ -\frac{(\ln x - \alpha)^2}{2\beta^2} \right] dx = F\left( \frac{\ln b - \alpha}{\beta} \right) - F\left( \frac{\ln a - \alpha}{\beta} \right) \] (3.19)

where \( F \) is the cumulative distribution function (CDF) of the standard normal distribution.

The PDF of the additional compliance \( H \) considering the distribution of the crack length is obtained using the fact that \( H \) is the monotonically increasing function of the crack length:

\[ f_{H}(H_{ij}) = \frac{1}{dH_{ij}} \frac{dC(c)}{dc} \] (3.20)

where discrete values of \( \frac{dH_{ij}}{dc} \) are obtained from the model analysis with various microcrack lengths, and the data are fit to a functional form to obtain a probability density function of additional compliance.

When the crack length has a certain distribution \( f_{C}(c) \), the evolution equation for the additional compliance (Eq. 3.12) becomes:

\[ H_{ij} = \frac{M}{\pi} \iint K_{ij}^{*} T_{ij} f_{C}(c) d\xi d\beta dc \] (3.21)

where the effect of the crack length variation is considered by spatial average process.

Similarly, the scatter in the experimental data of the fracture stress may be predicted through the PDF of the failure stress. When the PDF of the microcrack length is known and the grain size is assumed to be constant, the PDF of the failure stress is obtained by:

\[ f_{\Sigma}(\sigma_{f}) = \frac{1}{d\sigma_{f}} \frac{dC(c)}{dc} \] (3.22)
where \( \frac{d\sigma_f}{dc} \) is obtained from the model analysis.

### 3.3.2 Grain size variation

To know the grain size distribution in ice, the grain size histograms are constructed from thin section photographs of fresh water granular ice (Fig.3.3) and columnar S2 ice (Fig.3.4). Averaged grain sizes of 4.5 and 4.8 mm are obtained from the histograms although they are reduced to 4.2 and 4.6, respectively, when the histograms are fit into the Weibull distribution functions.

The CDF of the additional compliance which is now a function of the microcrack length and the grain size can be obtained by integrating the joint probability density function:

\[
F_H(\overline{H}_{ij}) = \int\int f_{c,D}(c,d) \, dc \, dd
\]

(3.23)

where the integration is performed in the domain of the crack length and the grain size that satisfy \( H_{ij}(c,d) \leq \overline{H}_{ij} \). The joint probability density function \( f_{c,D}(c,d) \) is obtained from the following relation:

\[
f_{c,D}(c,d) = f_{c|D}(c|d) f_D(d)
= f_c \left( \frac{c}{d} \right) \frac{f_D(d)}{d}
\]

(3.24)

The numerical evaluation of the cumulative density function, Eq. 3.23, is not easy to do, so in this study the PDF of the additional compliance is obtained from an approximate formulation. In a two-dimensional case, the crack length term can be separated from the expression of the additional compliance:
\[ H_{ij} = \kappa_{ij} c^2 \quad (3.25) \]

where \( \kappa_{ij} \) is the additional compliance divided by the square of the crack length. In the self-consistent model of Wu and Shyam Sunder (1992) the damaged compliance is used in the calculation of the additional compliance \( H_{ij} \), so the crack length term appears in the both sides of the Eq. 3.14 and \( \kappa_{ij} \) is the implicit function of the crack length. Because of this reason, the non-interactive model is used in this analysis, in which the additional compliance due to a crack nucleation is analyzed in a medium with the original compliance. The use of non-interactive model results in a little stiffer response of the material compared with the use of the self-consistent method.

With the CDF of the crack length distribution obtained from Eq. 3.15 and 3.17, the PDF of the additional compliance is calculated from probability theory as following:

\[
F_{H}(H_{ij}) = \int f_D(d) F_C(c) \, dc \, dd \\
= \int f_D(d) F_C \left( \frac{H_{ij}}{\kappa_{ij}} \right) \, dc \, dd
\quad (3.26)
\]

\[
f_{H}(H_{ij}) = \frac{d}{dH_{ij}} F_{H}(H_{ij})
\quad (3.27)
\]

where \( \kappa_{ij} \) is assumed to be the function of only the grain size \( d \) and should be calculated from the model analysis.

With the variation of the grain size and the crack length, the equation for the additional compliance is now modified to:

\[
H_{ij} = \frac{1}{\pi^2} \int \int \int M K_{kl} T_{kl} T_{ij} f_C(c) f_D(d) d \xi d \beta dc \, dd
\quad (3.28)
\]
In the above expression, the additional compliance is averaged over the possible range of the crack length and the grain size variation.

To obtain the PDF of failure stress considering the simultaneous distributions of crack length and the grain size is very difficult, so in this study the crack length is assumed to be proportional to the grain size. With such an assumption, the probability density function of the failure strength is obtained from the PDF of the grain size with the crack length proportional to the grain size:

\[
f_z(\sigma_f) = \frac{1}{d \sigma_f} f_D(d)
\]

(3.29)

3.3.3 Non-uniform distribution of basal plane and precursor orientation

It is widely acknowledged that the fabric orientation strongly influences the elastic moduli of ice (Nanthikesan and Shyam Sunder, 1993). In the granular ice, the basal plane is randomly distributed in all directions, so it is assumed in the calculation of the compliance that the basal plane and the precursor orientations are uniformly distributed on the two-dimensional plane. In columnar grained ice, three types of ice, S1, S2 and S3 ice, can be distinguished according to the basal plane orientation, although they contain identical single crystals. In S1 ice, the preferred crystallographic orientation of the c-axis is vertical, i.e., perpendicular to the ice cover. In S2 ice, the c-axis orientation is horizontal and randomly distributed. In the presence of strong currents, while the c-axis may still be located in the horizontal plane, a preferred orientation may develop. This type of ice is classified as S3 ice.

In general, the distribution of c-axis orientation is confined to a range of angles \(|\zeta_m - \psi| \leq \zeta \leq |\zeta_m + \psi|\) as shown in Fig. 3.5, where \(\zeta_m\) is the orientation of the mean c-
axis and $\Psi$ is the scatter angle. An appropriate PDF for idealization of the c-axis distribution is the symmetric beta distribution, which was used by Nanthikesan and Shyam Sunder (1992) to determine the elastic constants of S3 ice. The probability density function has the form:

$$f_Z(\zeta) = \frac{1}{B_n \pi^{2n+1}} [\zeta - (\zeta_m - \Psi)]^n [\zeta_m + \Psi - \zeta]^n \quad \text{for} \quad \zeta_m - \Psi \leq \zeta \leq \zeta_m + \Psi$$

$$= 0 \quad \text{elsewhere} \quad (3.30)$$

where $B_n = \frac{n!n!}{(2n+1)!}$

Fig. 3.6 shows an example of the beta distribution with $n=10$, the mean c-axis orientation $\zeta_m=\pi/2$ and the scatter angle $\Psi=\pi/2$

The original compliance of S3 ice can be computed after spatially averaging the value at each crystal orientation by multiplying the relative frequency of that orientation:

$$S_{ij} = \int S_{gij}(\zeta) f_Z(\zeta) d\zeta \quad (3.31)$$

where $S_{gij}$ is the compliance matrix of a single crystal with c-axis oriented at $\zeta$ in the local coordinate system, and $f_Z(\zeta)$ is the PDF of the c-axis orientation. The crystal elastic compliance at a given orientation can be determined by the following coordinate transformation of the matrix in the principal directions of the crystal:

$$S_g = R^T S_g R \quad (3.32)$$
where $\mathbf{R}$ is the rotation matrix based on the direction cosines of the c-axis, $\mathbf{R}^T$ is the transpose of the rotation matrix and $\mathbf{S}_g$ is the compliance matrix of a single crystal in the principal coordinate system (see Wu and Shyam Sunder, 1991).

An example of the plane stress compliance matrix of S3 ice is computed by the above method using $n=10$ at $T=-16^\circ\text{C}$ which is:

$$
\begin{bmatrix}
1.0773 & -0.2859 & 0 \\
-0.2859 & 0.9193 & 0 \\
0 & 0 & 2.9787
\end{bmatrix} \times 10^{-1}\text{GPa}^{-1}
\quad (3.33)
$$

Similarly, the compliance of S2 ice can be computed using the uniform distribution of basal plane orientation ($n=0$), which is:

$$
\begin{bmatrix}
1.0603 & -0.3539 & 0 \\
-0.3539 & 1.0603 & 0 \\
0 & 0 & 2.8286
\end{bmatrix} \times 10^{-1}\text{GPa}^{-1}
\quad (3.34)
$$

### 3.4 Numerical results

In this study, the statistical variation of the failure stress and the additional compliance caused by the variation of the underlying microstructural parameters are demonstrated through the 10 to 90th percentiles of the probability density functions. The distribution functions of the geometric parameters are obtained from experimental observation and are used as a weighting function in the computation of the total compliance. A simple probability theory is applied to the results from the model analysis to obtain the PDF's of the resulting failure stress and compliance.

Fig. 3.6 (a) and (b) show the numerically obtained PDF of failure stress and the appropriate fit by Weibull and lognormal density function. The probability densities are
obtained from Eq. 3.22 and Eq. 3.29 using various values of crack length and grain size. For the crack length distribution the PDF of the crack length is obtained from Eq. 3.17 with the grain size $d=4\text{mm}$, whereas the probability density function obtained from the grain size histogram is used for the grain size distribution case. In this case the crack length is taken to be 50% of the grain size. Fig. 3.7 shows the experimental data of the failure strength from Schulson (1990) and the analytical prediction using Eq. 3.13. The 10 to 90th percentiles obtained from the probability density functions are drawn in the same figure at the mean grain size of 4mm (crack length distribution) and 4.2mm (grain size distribution). The length of the percentiles is consistent with the scatter of the experimental data, but is not wide enough to comprise all the data. This implies that the scatter is caused by multiple sources, more than the crack length and the grain size.

Fig. 3.8 shows the evolution of the compliance in isotropic granular ice with (i) constant crack length and grain size, (ii) crack length variation with constant grain size, and (iii) both crack length and grain size variation. In case (i) and (ii), the grain size is set to 4.2 mm which is the mean value of the probability density function of the grain size determined from the grain size histogram (Fig. 3.3). In case (i), the crack length is determined from the mean value of the normalized crack length histogram (Fig. 3.2) which is 50% of the grain size. In case (ii), the PDF of crack length is determined from the normalized crack length histogram. For the last case, the PDF of the grain size as well as the PDF of the crack length is used in the computation of the evolution of the compliance. For each grain size the PDF of the crack length is constructed from the PDF of the normalized crack length (Eq. 3.17) and is weighted by the probability of the corresponding grain size. Similar computations are conducted with the S2 ice which has the original compliance of Eq. 3.34 (Fig. 3.9). The PDF of the grain size is also obtained from a thin section photograph of S2 ice. The results show that the increase of the compliance is larger in S2 ice. This may be explained by the fact that the grain size of the S2 ice is a little larger
than that of the granular ice, and the PDF of S2 ice is more skewed and widely spread than that of the granular ice.

Fig. 3.8 and 3.9 also display the 10 to 90th percentiles of the compliance obtained from the corresponding CDFs of the additional compliance. The length of the percentiles represents the amount of the scatter in compliance caused by the scatter in the material parameters. At the same loading condition the length is longer in S2 ice which has larger mean grain size and a more skewed and widely spread density function.

3.5 Conclusions

The following conclusions are drawn from the numerical simulation:
1. The 10 to 90th percentiles of the distribution function of the failure stress reasonably represent the scatter in experimental data.
2. The variations in the parameters generally fasten the evolution of the compliance.
3. The 10th to 90th percentiles of the compliance show that the range of distribution increases when the parameters are more scattered and skewed.
4. The damage accumulation in the columnar S3 ice can be predicted by applying the non-uniform distribution of the c-axis orientation in the evolution equation.
References

Cole, D. M. (1986), Effect of grain size on the internal fracturing of polycrystalline ice. CRREL REPORT 86-5, U.S. Army Cold Regions Research and Engineering Laboratory, Hanover, NH.


Fig. 3.1 Orientation of basal plane and precursor crack in an ice polycrystal
Fig. 3.2(a) Histogram of normalized crack length from Cole (1986), (b) Weibull distribution fit of the normalized crack length with the parameters $\alpha=1.4186$, $\beta=0.562$
Fig. 3.3 (a) Grain size histogram constructed from a thin section photograph of granular ice, (b) Weibull distribution fit of the grain size histogram.
Fig. 3.4(a) Grain size histogram of a S2 ice (constructed from a photograph in Sinha (1988)), (b) Weibull distribution fit of the histogram
Fig. 3.5 (a) Distribution of the c-axis (basal plane) orientation around the mean value ($\zeta_m$ is the orientation of the mean c-axis and $\Psi$ is the scatter angle), (b) Beta distribution of the c-axis distribution from 0 to $\pi$ with the distribution parameter $n=10$
Fig. 3.6 (a) Weibull distribution fit of the PDF of failure stress of granular ice considering crack length distribution at d=4mm (α=4.33 β=8.088), (b) Lognormal distribution fit considering grain size distribution with crack length proportional to the grain size (α=1.98, β=0.14)
Fig. 3.7 10 to 90th percentiles of failure stress distribution considering crack length and the grain size distribution
Fig. 3.8 Compliance evolution of granular ice with the 10 to 90th percentile of its distribution at $\sigma=6$ MPa
Fig. 3.9 Compliance evolution of S2 ice with the 10 to 90th percentile of distribution at σ=6 MPa
CHAPTER IV

MODELING OF THE BRITTLE FAILURE AND SPECIMEN SIZE EFFECT

Abstract

A micromechanical model is developed to predict the failure stress and specimen size effect of a polycrystalline ice. The elastic anisotropy mechanism is used to predict the nucleation of a microcrack from a precursor. The microstructural stress caused by the elastic anisotropy mechanism is added to the applied stress, and the combined stress field is used to analyze the nucleation and propagation of microcracks. The model takes into account the interaction between microcracks and between microcracks and specimen boundary. The model predictions of the failure stress fit the experimental data with reasonable accuracy, and follow the observation that the failure stress is inversely proportional to the square root of the mean grain size. Finally, the predicted failure stress increases as the size of the specimen increases. The size effect coefficients obtained by the model simulations fall between 1.6 to 5 with mean value of 2.7, which are comparable to the suggested value of 3 by Sanderson (1988) based on experimental data.

4.1 Introduction

Ice becomes brittle as the strain rate goes higher than the ductile-brittle transition point. The experimental data for the failure stress of polycrystalline ice have been previously obtained by Gold (1972), Cole (1985) and Schulson (1990). According to the results, the stress-strain relationship of ice under the strain rate of less than about $10^{-4}$ s$^{-1}$ is characterized by the ascending and descending branch, whereas only the ascending branch is obtained at the strain rate greater than about $10^{-3}$ s$^{-1}$. At the high end of the ductile-to-
brittle transition, the failure of ice is associated with the distributed cracking activity and the extension of localized microcracks leading to compressive failure by shear faulting and axial splitting. Ice generally fails by axial splitting when appropriately located cracks propagate rapidly throughout the specimen. Shear faulting occurs under the biaxial compression, where the nucleated cracks link together to form a localized shear band.

It is widely recognized that a brittle material shows a size effect; in particular the failure stress decrease as the specimen size increases. In ice, Kry (1979) and Iyer (1983) found a pronounced scale-effect when ice interacts with structures. The pressure area map constructed by Sanderson (1988) from a large range of experimental data on the indentation strength of ice indicates that the peak pressures measured over small areas such as tested in the laboratory are higher than those obtained from large-scale indentation tests (Fig. 4.1).

The scale effect in brittle materials is generally caused by the existence of internal cracks. Sanderson (1988) specified the theoretical background of the scale effects in brittle ice two ways: the contributions based on fracture mechanics and Weibull type statistics. If a sample is scaled up geometrically by a factor $r$ including the size of the internal cracks (Fig. 4.2(a)), then from a basic fracture mechanics argument the fracture strength decreases by a factor $r^{-1/2}$. This result is based on the assumption that a larger sample contains larger cracks. But in the case of ice grown in a laboratory, where it is possible to control the size of grains (and thereby the size of internal cracks), this assumption may not be valid. Nevertheless the fracture mechanics based size effect is an important cause of the phenomenon observed in the field. There is another source of scale effect based on the assumption that a material contains a statistical population of cracks of various sizes, and a large specimen has greater possibility of having large cracks (Fig. 4.2(b)). This argument was first proposed for tensile fracture where the weakest link concept applies and a single crack propagation leads to sudden failure. However, as noted by Schulson and Zhang (1990), it may be reasonable to apply the same assumption to the compressive failure because of the following reason: The brittle compressive failure of ice is associated with
the formation of wing cracks which are formed by local tensile fracture, and the failure is initiated by the unstable propagation of single crack or by the subsequent linkage of cracks. Considering this statistical effects the failure stress is represented by:

\[
\frac{\sigma_{f2}}{\sigma_{f1}} = \left( \frac{V_2}{V_1} \right)^{\frac{1}{m}}
\]

where \(\sigma_{f1}\) and \(\sigma_{f2}\) are the failure stresses for samples of volume \(V_1\) and \(V_2\), respectively, and \(m\) is the Weibull modulus. Sanderson (1988) proposed 3 for this parameter based on the pressure area map, and Schulson and Zhang (1990) proposed 6 after reviewing the values for other brittle materials.

In a large-scale indentation, non-simultaneous failure is the most dominant mechanism for the size effect phenomenon (Kry, 1980; Sanderson, 1986). The idea of the non-simultaneous failure is based on the hypothesis that large scale failure occurs by successive fracture of independent zones, and the failure stress is dependent on the failure of small cells instead of the failure of whole ice plate.

To study the effect of specimen size on the prediction of brittle compressive failure stress of ice, we need a method to; (i) generate random microstructures of ice in different scales, and (ii) analyze the finite sized ice specimens with internal cracks. In this research a graph representation method is used to construct a random microstructure of polycrystalline ice. The method has been applied by Ostoja-Starzewski (1987), Frost and Thompson (1987) and Wu and Niu (1995). The graph model provides a basis for defining the geometrical randomness of the crack location and orientation. Typical microstructure of ice simulated from the graph model is shown in Fig. 4.3.

Once the size and the macrostructure of an ice specimen is defined, the boundary force method (BFM), which is a form of an indirect boundary element method, is used to analyze finite sized ice specimen with growing number of cracks. Tan and Bigelow (1989)
have applied the method to compute the stress intensity factors of anisotropic graphite/epoxy laminates with single cracks. They included a moment in addition to the concentrated normal and shear forces in the orthotropic formulation of the BFM. Wu (1993a,b) has used the technique to estimate the stress intensity factors and the effective moduli of arbitrarily located multiple cracks in a finite anisotropic media. The method of analysis is based on the BFM to simulate the effect of the boundary and on the approximate technique for interactions between cracks. Both depend on the superposition schemes which can be simultaneously applied to analyze the interacting cracks in finite media. In this research the analytical approach of Wu (1993) will be followed to predict the failure stress of different sized specimens of polycrystalline ice.

4.2 Model formulation

4.2.1 Graph representation of a random microstructure

In this research the microstructure of ice is represented by two dimensional tessellation of Voronoi polygons following the approach of Wu and Niu (1995). The process of constructing the tessellation is as following: A set of $n$ points are randomly deposited in a two-dimensional plane and the sets of regions around those points constitute a set of Voronoi polygons. If a location is equidistant from two points, then the location is on the boundary of two adjacent polygons. Once the shape and location of each grain is generated, the c-axis orientation of each grain and the location of the precursor (a small starter crack located at triple points) are randomly assigned.

4.2.2 Nucleation of microcracks
Shyam Sunder and Wu (1990) postulated that a microcrack nucleates from a precursor located at a grain boundary triple point. The assumption is based on the idea that stress singularities can be induced at grain boundary junctions as a result of a polycrystal thermal or elastic expansion anisotropy (Evans, 1978). These stress-induced flaws are named precursors and are assumed to be 10 to 20 % of grain size in length. For a first-order analysis, the stress singularity plays the role of precursor formation and are neglected in the subsequent analysis of crack nucleation and propagation.

The elastic anisotropy mechanism, which is believed to be dominant at high strain rates, stems from the incompatible deformation of the differently oriented crystals. Because of the elastic property mismatch, the differently oriented constituent crystals tend to deform incompatibly. Since this incompatibility is not realized in the polycrystal, the microstructural stresses are generated. The microstructural stress can be positive or negative depending on the crystal orientation and the external loading. Consider a precursor of length $2a$ with orientation $\beta$ and grains around it with randomly oriented basal planes as shown in Fig. 4.4. The microstructural stress $\sigma_o$ can be estimated by (Shyam Sunder and Wu, 1991):

$$\sigma_o = \frac{1}{2} \left[ \left( C_g(\zeta_1) + C_g(\zeta_2) \right) S - 2I \right] \sigma_a \quad (4.2)$$

where $C_g$, $S$ and $\sigma_a$ are the elastic stiffness of single ice crystal dependent on the basal plain orientation $\zeta$, the compliance of the polycrystallin ice and the applied stress, respectively.

In this study the effect of the specimen boundary is not considered in the analysis of the crack nucleation from precursors. This simplification may not affect the failure stress of ice since the final failure occurs after significant damage has been progressed (Shyam Sunder et. al., 1995) and the order of nucleation may not be important. With the consideration of the microstructural stress the total stress around a precursor becomes:
\[ \sigma = \sigma_o + \sigma_a \]  \hspace{2cm} (4.3)

If a local Cartesian coordinate \(x-y\) is defined such that the plane of the precursor lies parallel to the \(x\) axis, the stress field ahead of a precursor is characterized by the mode I and mode II stress intensity factors, which are:

\[ K_I = \sigma'_{yy} \sqrt{\pi a} \]  \hspace{2cm} (4.4)

\[ K_{II} = \sigma'_{xy} \sqrt{\pi a} \]  \hspace{2cm} (4.5)

where \(\sigma'_{yy}\) and \(\sigma'_{xy}\) are the normal and effective shear stress represented in the local precursor coordinate, respectively, and \(a\) is the half precursor length. The effective shear stress is set to zero when the applied shear stress is smaller than or equal to the magnitude of the compressive normal stress multiplied by the friction coefficient. The precursor nucleates into a microcrack when the maximum principal tensile stress criterion of Erdogan and Sih (1963) is satisfied, and the nucleation criterion becomes:

\[ K_I \cos^3 \frac{\theta_m}{2} - 3K_{II} \cos^2 \frac{\theta_m}{2} \sin \frac{\theta_m}{2} = k_{IC} \]  \hspace{2cm} (4.6)

where \(\theta_m\) is the angle that makes the asymptotic distribution of the shear stress equal to zero and is given by:

\[ \tan \frac{\theta_m}{2} = \frac{1}{4} \left[ \frac{K_I}{K_{II}} \pm \sqrt{\left( \frac{K_I}{K_{II}} \right)^2 + 8} \right] \]  \hspace{2cm} (4.7)
The microstructural fracture toughness $k_{IC}$ is determined from the effective surface energy $\gamma$, the Young's modulus $E$, and the Poisson's ratio $\nu$:

$$k_{IC} = \sqrt{2E\gamma} \quad \text{plane stress}$$

$$k_{IC} = \sqrt{\frac{2E\gamma}{1-\nu^2}} \quad \text{plane strain} \quad (4.8)$$

Once the criterion is satisfied, a precursor nucleates into a microcrack which grows toward the direction of maximum tensile stress as the loading increases. In this study it is assumed that the precursor directly grows into its final configuration at the moment that the criterion is satisfied. 50% of the average grain size is taken to be the final microcrack length based on the experimental observation of Cole (1986).

4.2.3 Failure of ice

Once a crack nucleates from a precursor the stress intensity factors at the tips of the cracks can be obtained by simultaneous application of two superposition schemes (Wu, 1993). In the first superposition scheme, concentrated forces and couples acting on an imaginary boundary within an infinite medium are superposed to transform the problem of a finite cracked medium to that of an infinite cracked medium. In the second scheme, tractions acting on crack lines are superposed to compute the stress field around each crack.

Superposition of concentrated forces and couples

The boundary force method of Tan and Bigelow (1989) is used to obtain the solution to the boundary value problem by using the superposition of the fundamental solutions for concentrated forces and moments acting on the trace of external boundary.
Let's consider a finite specimen with arbitrary number of cracks with uniform uniaxial compression (Fig. 4.5(a)). The finite specimen can be replaced by the superposition of the \( V \) configurations with initially unknown concentrated forces and a couple on each of \( V \) boundary elements. The concentrated forces \( X_{\mu \nu} (\mu=1,3; \nu=1, V) \) are applied at a small distance on the outward normal from the mid-point of the boundary elements to avoid the singularities in the computations of the stresses on the boundary. Note that \( X_{1 \nu} \) and \( X_{2 \nu} \) denote forces in the \( x_1 \) and \( x_2 \) directions, respectively, and \( X_{3 \nu} \) denotes a concentrated couple. The concentrated forces induce stresses on the boundary elements, and the induced stresses yield resultant forces after the superposition. The resultant forces are equated to the prescribed external loads \( B_{ij} (i=1,3; j=1, V) \) to obtain the magnitude of the initially unknown concentrated forces. As a result of the superposition scheme, the resultant stress and displacement field within the imaginary boundary are approximately equal to those within the actual specimen. If we denote \( A_{ij}^{\mu \nu} \) the \( i \)-type force acting on the \( j \)th boundary element due to the application of the \( u \)-type force of unit magnitude acting at the \( \nu \)th boundary element, then the prescribed loads can be expressed as:

\[
B_{ij} = \sum_{\mu=1}^{3} \sum_{\nu=1}^{V} A_{ij}^{\mu \nu} X_{\mu \nu} \quad (4.9)
\]

The unknown forces \( X_{\mu \nu} \) is obtained from solving above equation. The influence force \( A_{ij}^{\mu \nu} \) can be calculated from stress fields due to concentrated forces in an infinite medium.

**Superposition of crack line traction**

In this scheme the fundamental solutions for the stress fields in \( V \) sub-problems with interacting cracks will be estimated by superposition. Fig. 4.5(b) shows the decomposition of each of the \( V \) sub-problems to \( M \) problems each involving a single crack plus a homogeneous problem with no crack. The unknown normal and shear tractions at \( a-\)
th crack caused by a unit \( u \)-type force at \( v \)th boundary element are denoted by \( u_v p_{\alpha}(x^\alpha) \) and \( u_v q_{\alpha}(x^\alpha) \), respectively, and can be approximated by a series of Legendre polynomials:

\[
_{u_v}p_{\alpha}(x^\alpha) = \sum_{n=0}^{N} \frac{a_n}{u_v} L_n(\xi_{\alpha})
\]

\[
_{u_v}q_{\alpha}(x^\alpha) = \sum_{n=0}^{N} \frac{b_n}{u_v} L_n(\xi_{\alpha})
\]

(4.10)

(4.11)

where \( \xi_{\alpha} \) is the local crack coordinate normalized by the half crack length \( c_\alpha \), and the Legendre polynomial \( L_n \) is:

\[
L_n = \frac{1}{2^n} \frac{d^n}{d\xi_{\alpha}^n} \left( \xi_{\alpha}^2 - 1 \right)^n, \quad \xi_{\alpha} = \frac{x^\alpha}{c_\alpha}
\]

(4.12)

If \( \alpha^\beta g_n(\alpha x) \) and \( \alpha^\beta h_n(\alpha x) \) denote the normal stresses induced at the \( \alpha \)th crack by a normal and shear traction of the form \(-L_n(\xi_{\beta})\) applied at the \( \beta \)th crack, respectively, then the sum of: (i) the unknown normal traction \( u_v p_{\alpha}(\alpha x) \), (ii) the normal traction induced on the crack line by the unknown tractions on all other isolated cracks, and (iii) the normal traction induced on the crack line by a unit \( u \)-type force acting at the \( v \)th boundary element \( u_v p_A(\alpha x) \), is zero since the crack faces are traction free:

\[
\sum_{n=0}^{N} \frac{a_n}{u_v} L_n(\xi_{\alpha}) + \sum_{\beta=1}^{M} \sum_{n=0}^{N} \frac{b_n}{u_v} L_n(\xi_{\alpha}) + \sum_{\beta=1}^{M} \sum_{n=0}^{N} \frac{b_n}{u_v} \alpha^\beta h_n(\alpha x) + \sum_{\beta=1}^{M} \sum_{n=0}^{N} \frac{b_n}{u_v} \alpha^\beta h_n(\alpha x) + \sum_{u_v}^{A} p_A(\alpha x) = 0
\]

(4.13)

These \( M \) equations are multiplied by \( L_j(\xi_{\alpha}) \), \( j=0,1,...,N \) and integrated with respect to \( \alpha x \) to yield a system of \( M(N+1) \) equations:
\[
\sum_{\beta=bn}^{M} \sum_{\omega}^{N} \left[ \omega^{\alpha_{\beta}} \left( \alpha x \right) L_{j}(\xi_{\alpha}) d^{\alpha x} + \omega^{\beta_{\alpha}} \left( \alpha \right) L_{j}(\xi_{\alpha}) d^{\alpha x} \right] - \frac{2c_{\alpha}}{2j+1} \omega^{\alpha_{j}} + \int_{c_{\alpha}}^{c_{\alpha}} \omega^{pA} \left( \alpha x \right) L_{j}(\xi_{\alpha}) d^{\alpha x} = 0
\] (4.14)

Note that the property of the orthogonality of the Legendre polynomials are used to produce the above equations. The corresponding equations for the superposition of the shear tractions can be similarly obtained:

\[
\sum_{\beta=bn}^{M} \sum_{\omega}^{N} \left[ \omega^{\alpha_{\beta}} \left( \alpha x \right) L_{j}(\xi_{\alpha}) d^{\alpha x} + \omega^{\beta_{\alpha}} \left( \alpha \right) L_{j}(\xi_{\alpha}) d^{\alpha x} \right] - \frac{2c_{\alpha}}{2j+1} \omega^{b_{j}} + \int_{c_{\alpha}}^{c_{\alpha}} \omega^{qA} \left( \alpha x \right) L_{j}(\xi_{\alpha}) d^{\alpha x} = 0
\] (4.15)

In the above equations, the tractions \( \omega^{\alpha g_{n}} \), \( \omega^{\beta h_{n}} \), \( \omega^{\alpha r_{n}} \), and \( \omega^{\beta s_{n}} \) are obtained from the stress field caused by the normal and shear tractions on the cracks, and \( \omega^{pA} \left( \alpha x \right) \) and \( \omega^{qA} \left( \alpha x \right) \) are obtained from the stress field due to the unit concentrated forces on every boundary element. If a local Cartesian frame \((x,y)\) is attached to the center of a single crack of length \(2l\), the elastic stress fields in a two-dimensional medium can be obtained from a pair of analytical stress functions \( \varphi(z_{1}) \) and \( \psi(z_{2}) \):

\[
\sigma_{11} = 2 \text{Re} \left[ \mu_{1}^{2} \varphi'(z_{1}) + \mu_{2}^{2} \psi'(z_{2}) \right] \quad \text{(4.16)}
\]
\[
\sigma_{22} = 2 \text{Re} \left[ \varphi'(z_{1}) + \psi'(z_{2}) \right] \quad \text{(4.17)}
\]
\[
\sigma_{12} = -2 \text{Re} \left[ \mu_{1} \varphi'(z_{1}) + \mu_{2} \psi'(z_{2}) \right] \quad \text{(4.18)}
\]

where \( z_{1} = x + \mu_{1} y, \quad z_{2} = x + \mu_{2} y, \) and the complex parameters \( \mu_{1}, \mu_{2} \) and their complex conjugates are complex roots of the characteristic equation.
\[ S_{11} \mu^4 - 2S_{26} \mu^3 + (2S_{12} + S_{66})\mu^2 - 2S_{26} \mu + S_{22} = 0 \]  \hspace{1cm} (4.19)

where \( S_{ij}; i, j = 1, 2, 6 \) are the elements of the compliance matrix of the anisotropic medium. Since the tractions acting on the cracks consist of the sum of polynomial functions, the induced stress fields can be obtained by adding those due to the elementary functions with the form \(-(x/c)^n; n = 0, 1, 2, ..., N\). The appropriate stress functions for the polynomial elementary functions can be found in Wu (1993), and those for the stress fields resulting from the application of the three concentrated forces in an uncracked infinite medium can be found in Lekhnitskii (1986) and Tan and Bigelow (1989). For completeness, those stress functions are given in the appendix.

After the coefficients are obtained, the stress distribution on all boundaries, due to the application of a \( u \)-type force of unit magnitude acting on \( v \)th boundary element in the cracked medium, can be estimated by superposing the single crack problems and the homogeneous problem. The stress distributions along the boundary elements are integrated to yield the resultant forces \( B_{ij} \). The concentrated loads \( X_{uv} \), which are required to be applied to the decomposed configurations (Fig. 4.5), can be obtained from solving Eq. 4.9. Then \( X_{uv} \) are multiplied to the coefficients \( \alpha_{uv}a_n \) and \( \alpha_{uv}b_n \), which result from applying unit concentrated loads, and superposition of all the configurations in Fig. 4.5 is used to get the coefficients for the total tractions acting on the \( \alpha \)th crack:

\[ \alpha_{a_n} = \sum_{u=1}^{3} \sum_{v=1}^{V} \alpha_{uv}a_n X_{uv} \]  \hspace{1cm} (4.20)

\[ \alpha_{b_n} = \sum_{u=1}^{3} \sum_{v=1}^{V} \alpha_{uv}b_n X_{uv} \]  \hspace{1cm} (4.21)

**Computation of stress intensity factors**
The mode I and mode II stress intensity factors at the tips of the cracks can be obtained by:

\[ K_I^\pm = -\frac{1}{\sqrt{\pi c_\alpha}} \int_{c_\alpha}^{c_\alpha \pm c_\alpha} -P_\alpha(\alpha x) \sqrt{\frac{c_\alpha^2 - \alpha^2 x^2}{c_\alpha^2 + \alpha^2 x^2}} \, d\alpha x \]  
(4.22)

\[ K_{II}^\pm = -\frac{1}{\sqrt{\pi l_\alpha}} \int_{c_\alpha}^{c_\alpha \pm c_\alpha} -Q_\alpha(\alpha x) \sqrt{\frac{c_\alpha^2 - \alpha^2 x^2}{c_\alpha^2 + \alpha^2 x^2}} \, d\alpha x \]  
(4.23)

where \( p_\alpha \) and \( q_\alpha \) are expressed by:

\[ p_\alpha = \sum_{u=1}^{3} \sum_{v=1}^{V} \sum_{n=1}^{N} a_{uv} X_{uv} L_n(\xi_\alpha) \]  
(4.24)

\[ q_\alpha = \sum_{u=1}^{3} \sum_{v=1}^{V} \sum_{n=1}^{N} b_{uv} X_{uv} L_n(\xi_\alpha) \]  
(4.25)

It is known that reasonably accurate results can be obtained for the stress intensity factors if the polynomial include terms up to the quadratic, i.e., \( N=2 \) (Wu, 1993). Wu (1993) also shows that the stress intensity factors increase as the cracks are located closer to the boundary of the specimen, and the stress intensity factor at the crack tip closer to the boundary is greater than that of the other crack tip.

In this study the maximum principal tensile stress criterion is used again to predict failure of ice, except the macroscopic fracture toughness is used in this case:

\[ K_I \cos^3 \frac{\theta_m}{2} - 3K_{II} \cos^3 \frac{\theta_m}{2} \sin \frac{\theta_m}{2} = K_{IC} \]  
(4.26)
$K_I$ and $K_{II}$ are the mode I and mode II stress intensity factors of the microcrack, respectively, and $K_{IC}$ is the macroscopic fracture toughness. The above criterion was successfully used in prediction of the failure stress of ice by Shyam Sunder et. al. (1995).

4.3 Material parameters

The compliance matrix of a single ice crystal determined by Gammon et al. (1983) at temperature $T=-16^\circ C$ are given as follows:

\[
\begin{bmatrix}
1.0318 & -0.2316 & -0.4287 \\
0.8441 & -0.2316 & 0 \\
1.0318 & & \\
\end{bmatrix}
\begin{bmatrix}
sym. & 3.3179 \\
& 2.9210 \\
& & 3.3179 \\
\end{bmatrix}
\]

\[10^{-1}\text{GPa}^{-1}\] (4.27)

where the plane of transverse isotropy is contained in the $X_1$-$X_3$ plane, and the $c$-axis is in the $X_2$ direction. The elastic constants of polycrystalline ice are determined by the distribution of the crystallographic orientation of each grain. The undamaged compliance matrix of isotropic granular ice at $-16^\circ C$ are (Gammon et al. (1983)):

\[
\begin{bmatrix}
1.0716 & -0.3486 & -0.3486 \\
1.0716 & -0.3486 & 0 \\
1.0716 & & \\
\end{bmatrix}
\begin{bmatrix}
sym. & 2.8401 \\
& 2.8401 \\
& & 2.8401 \\
\end{bmatrix}
\]

\[10^{-1}\text{GPa}^{-1}\] (4.28)

The corresponding stiffness matrices can be obtained by inverting the compliance matrices. The above 3-D matrices can be transformed into plane strain matrices using the relation
given by Savin (1961). The transformed plain strain components of the compliance matrix of the single ice crystal and polycrystalline ice become:

\[
\begin{bmatrix}
0.8537 & -0.3278 & 0 \\
0.7921 & 0 & 10^{-1} \text{GPa}^{-1} \\
\text{sym} & 3.3179 \\
\end{bmatrix}
\]  \hspace{1cm} (4.29)

\[
\begin{bmatrix}
0.9582 & -0.4620 & 0 \\
0.9582 & 0 & 10^{-1} \text{GPa}^{-1} \\
\text{sym} & 2.8401 \\
\end{bmatrix}
\]  \hspace{1cm} (4.30)

For the transversely isotropic polycrystalline ice under plane strain condition, the Young's modulus \(E\) is 9.369 GPa, the shear modulus \(G\) is 3.535 GPa, and the Poison ratio is 0.325. The surface energy \(\gamma\) is taken from Ketcham and Hobbs (1969) to be 0.0765 J/m\(^2\).

The macroscopic fracture toughness varies from about 0.08 to 0.12 MPam\(^{0.5}\) depending on temperature (Nixon and Shulson, 1986). The friction coefficient between crack surfaces is the function of strain rate and temperature (Schulson, 1990). In ductile-brittle transition and brittle region the value varies between 0.15 and 0.6 depending on temperature and strain rate.

4.4 Numerical results

In this study four specimens with different ice microstructures are generated for analysis. The specimens are 35×35 mm in size and have mean grain size of about 5 mm. Based on these data sets for initial configurations (which have mean grain size of 5 mm) new data sets of ice specimens with different mean grain size can be obtained by multiplying appropriate constants to the data sets of original configurations. In this way specimens with various grain sizes ranging from 2 to 8 mm are prepared from each original
microstructure, and they are used to predict failure stress. The resultant specimen and grain sizes obtained from the original data set A are summarized in Table 4.1. The effect of the boundaries in finite specimens is considered by the boundary force method. In each case the specimen boundaries are divided into 120 elements to simulate the boundary effect, which is enough to ensure convergence of the stress intensity factor (Wu, 1993). The distance from the boundary elements to the point of loading is taken to be the same as the length of the boundary element to prevent the singularity. The maximum principal tensile stress criterion is applied to predict the failure stress, and the results are shown in Fig. 4.6 where the numerical results are compared with the experimental data of Schulson (1990). In Fig. 4.6(a) the experimental data are obtained at -10°C at the strain rate of 10⁻³s⁻¹. In the simulation the friction coefficient is taken to be 0.5 based on Schulson (1990) and the macroscopic fracture toughness of 80 KPa m⁰.⁵ is taken from Nixon and Schulson (1987). Fig. 4.6(b) shows the experimental data for the failure stress obtained at T= -10°C and ε=10⁻¹s⁻¹ and the model prediction using the friction coefficient of 0.15 and the fracture toughness of 80 KPa m⁰.⁵. The model predictions reasonably agree with the experimental data and follow the experimental trend that the failure stress is inversely proportional to the square root of the grain size. Shyam Sunder et. al. (1995) predicted the brittle failure stress of ice using the self-consistent method in an infinite medium, considering every crack oriented from zero to π. Compared with their results, the present results generally form a lower bound since the stress intensity factors at the tip of the cracks are greater than those obtained at an infinite medium as a result of the boundary effects and the crack-crack interaction.

To simulate the size effects, parts of the specimens are cut off from the initial 35×35 mm specimens to make smaller sub-specimens without greatly changing the mean grain size. In this way, four sets of sub-specimens with the size of 30×30, 25×25, and 20×20 mm are prepared from each of the four original data sets for analysis. Fig. 4.7 shows the failure stresses obtained from the analysis of the sub-specimens. Table 4.2
summarizes the size of the sub-specimens obtained from the original data set A and the corresponding failure stress. The linear regression method is used to obtain the size effect coefficient $m$ for each data set. The obtained coefficients range from 1.6 to 5, with the mean value of 2.7. These values are reasonable compared with the value $m=3$ suggested by Sanderson (1988).

Fig. 4.8 shows the critical crack densities at failure for differently sized specimens. The crack density is defined as sum of the square of the cracks divided by the specimen area. It is shown that the predicted crack density at failure increases as the specimen size decreases. This is natural considering the observation that a smaller specimen fails at higher stress.

4.5 Conclusion

In this study the failure strength and the specimen size effect of brittle ice is predicted by a micromechanical model. The microstructure of a polycrystalline ice is simulated using the graph model. Interactions between cracks as well as between cracks and boundary elements are considered in the analysis. The final failure is predicted by maximum principal stress criterion. The findings from this research are as following:

1. The failure stress predicted by the model fits the experimental data with reasonable accuracy.
2. The predicted failure stress is proportional to the inverse of the square root of the grain size, which agrees with the experimental observation.
3. The scatter of the failure stress frequently observed in experimental data may be explained by the model prediction using different microstructures of ice with the same mean grain size.
4. The failure stress obtained from the model increases as the size of the specimen decreases. The size effect parameters obtained from model simulations are within or close to the values obtained from the experimental data.

5. The critical crack density at failure increases as the size of the specimen decreases.
Appendix

Stress functions for the elementary polynomial functions

If \( p\varphi_n(z_1) \) and \( p\psi_n(z_2) \) denote the stress functions due to normal tractions \(-(x/c)^n; n = 0, 1, 2, ..., N\) on the crack, and if \( q\varphi_n(z_1) \) and \( q\psi_n(z_2) \) denote the stress functions due to shear tractions of the same functional forms, then the derivatives of these functions for \( n = 0, 1, 2 \) become:

\[
p\varphi'_0 = -\frac{\mu_2}{\mu_1 - \mu_2} \frac{z_1 - (z_1^2 - c^2)^{1/2}}{2c(z_1^2 - c^2)^{1/2}};
\]

\[
p\psi'_0 = \frac{\mu_1}{\mu_1 - \mu_2} \frac{z_2 - (z_2^2 - c^2)^{1/2}}{2(z_2^2 - c^2)^{1/2}}
\]

\[
p\varphi'_1 = -\frac{\mu_2}{\mu_1 - \mu_2} \frac{z_1^2 - z_1(z_1^2 - c^2)^{1/2} - \frac{c^2}{2}}{2c(z_1^2 - c^2)^{1/2}}
\]

\[
p\psi'_1 = \frac{\mu_1}{\mu_1 - \mu_2} \frac{z_2^2 - z_2(z_2^2 - c^2)^{1/2} - \frac{c^2}{2}}{2c(z_2^2 - c^2)^{1/2}}
\]

\[
p\varphi'_2 = -\frac{\mu_1}{\mu_1 - \mu_2} \frac{z_1^3 - z_1^2(z_1^2 - c^2)^{1/2} - \frac{z_1c^2}{2}}{2c^2(z_1^2 - c^2)^{1/2}}
\]

\[
p\psi'_2 = \frac{\mu_1}{\mu_1 - \mu_2} \frac{z_2^3 - z_2^2(z_2^2 - c^2)^{1/2} - \frac{z_2c^2}{2}}{2c^2(z_2^2 - c^2)^{1/2}}
\]

\[
q\varphi'_n(z_1) = \frac{p\varphi'_n(z_1)}{\mu_2}; \quad q\psi'_n(z_2) = \frac{p\psi'_n(z_2)}{\mu_1}
\]

Stress functions for the three concentrated forces

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The stress functions for the unit forces in the \(x_1-x_2\) directions can be written as:

\[
\varphi^\prime(z_1) = \frac{A_u}{z_1}; \quad \psi^\prime(z_2) = \frac{B_u}{z_2}
\]  

where

\[
A_1 = \frac{\mu_1}{2\pi i(\mu_1 - \mu_2)(\mu_1 - \bar{\mu}_2)(\mu_1 - \bar{\mu}_1)}\left(\frac{\bar{\mu}_1 + \mu_2 + \mu_2 - \frac{S_{16}}{S_{11}} - \mu_2\bar{\mu}_1\bar{\mu}_2}{S_{12}}\right)
\]  

\[
A_2 = \frac{\mu_1}{2\pi i(\mu_1 - \mu_2)(\mu_1 - \bar{\mu}_2)(\mu_1 - \bar{\mu}_1)}\left(\frac{\bar{\mu}_1(\bar{\mu}_2 + \mu_2) - \frac{S_{12}}{S_{11}} - \mu_2\bar{\mu}_1\bar{\mu}_2}{S_{22}}\right)
\]  

\[
B_1 = \frac{\mu_2}{2\pi i(\mu_1 - \mu_2)(\mu_1 - \bar{\mu}_2)(\mu_2 - \bar{\mu}_2)}\left(\frac{\bar{\mu}_2 + \mu_1 + \mu_1 - \frac{S_{16}}{S_{11}} - \mu_1\bar{\mu}_1\bar{\mu}_2}{S_{12}}\right)
\]  

\[
B_2 = \frac{\mu_2}{2\pi i(\mu_1 - \mu_2)(\mu_1 - \bar{\mu}_2)(\mu_2 - \bar{\mu}_2)}\left(\frac{\bar{\mu}_2(\bar{\mu}_1 + \mu_1) - \frac{S_{12}}{S_{11}} - \mu_1\bar{\mu}_1\bar{\mu}_2}{S_{22}}\right)
\]

The stress functions for the stress fields resulting from the application of a unit counterclockwise couple in an uncracked infinite plate are given by:

\[
3\varphi^\prime(z_1) = \frac{1}{2} (\mu_1 A_1 - A_2); \quad 3\psi^\prime(z_2) = \frac{1}{2} (\mu_2 B_1 - B_2)
\]  

(A4.13)
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Table 4.1  Failure stress of ice specimens prepared from the data set A: the data set for the original 5 by 5 mm specimen is multiplied by various constants to reduce or enlarge the size of the specimen.

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Size of specimen (mm)</th>
<th>Mean grain size (mm)</th>
<th>Failure stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(i)</td>
<td>14×14</td>
<td>2</td>
<td>10.7</td>
</tr>
<tr>
<td>(ii)</td>
<td>21×21</td>
<td>3</td>
<td>8.8</td>
</tr>
<tr>
<td>(iii)</td>
<td>35×35</td>
<td>5</td>
<td>6.6</td>
</tr>
<tr>
<td>(iv)</td>
<td>49×49</td>
<td>7</td>
<td>5.7</td>
</tr>
<tr>
<td>(v)</td>
<td>56×56</td>
<td>8</td>
<td>5.0</td>
</tr>
</tbody>
</table>

Table 4.2. Failure stress of specimens prepared from data set A by cutting off part of the original specimen.

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Size of specimen (mm)</th>
<th>Mean grain size (mm)</th>
<th>Failure stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(I)</td>
<td>35×35</td>
<td>5</td>
<td>6.6</td>
</tr>
<tr>
<td>(II)</td>
<td>30×30</td>
<td>~5</td>
<td>7.2</td>
</tr>
<tr>
<td>(III)</td>
<td>25×25</td>
<td>~5</td>
<td>8.0</td>
</tr>
<tr>
<td>(IV)</td>
<td>20×20</td>
<td>~5</td>
<td>8.3</td>
</tr>
</tbody>
</table>
Fig. 4.1 A pressure-area curve for ice (Sanderson, 1988).
Fig. 4.2 Scaling assumptions: (a) geometric scaling of specimen size and crack length; (b) scaling of specimen size and statistical distribution of flaws.
Fig. 4.3 Typical microstructure of ice generated by the graph representation method.
Fig. 4.4 Precursor and basal plane orientation.
Fig. 4.5 Decomposition of the problem of a finite cracked medium into problems in infinite media: (a) superposition of concentrated forces and couples; (b) superposition of crack line tractions.
Fig. 4.6 Prediction of the failure strength of ice: (a) prediction of the experimental data obtained at $\dot{\varepsilon}=10^{-3}\text{s}^{-1}$ at $T=-10^\circ\text{C}$
Fig. 4.6 (b) prediction of the experimental data obtained at $\dot{\varepsilon}=10^{-1}\text{s}^{-1}$ at $T=-10^\circ\text{C}$
Fig. 4.7 Crack densities at failure obtained from: (a) data set A; (b) data set B
Fig. 4.7 Crack densities at failure obtained from: (c) data set C; (d) data set D
Fig. 4.8 Prediction of size effect coefficient from four data sets
CHAPTER V

MICROMECHANICAL MODEL OF ICE IN THE DUCTILE-TO-BRITTLE TRANSITION

Abstract

In this study a micromechanical model is proposed to predict the behavior of polycrystalline ice in the ductile to brittle transition domain. The grain boundary dislocation pileup mechanism of Wu and Niu (1995) is used for microcrack nucleation at a grain boundary triple point. According to the mechanism a microcrack nucleates when the energy of the pileup group becomes larger than the energy of the crack system. The microstructural stress caused by the elastic property mismatch between ice crystals is added to the stress from remote loading in the formulation of crack nucleation and growth. The nucleated microcracks are assumed to form grain boundary cracks with the length of grain boundary facet, and grow further into the crystals to form wing cracks. The maximum principal tensile stress criterion is used to decide the nucleation of grain boundary cracks and wing cracks. The grain boundary crack-wing crack combination is approximated with a straight crack with a point force in calculation of the stress intensity factor and the evolution of compliance. The effect of creep is included in the computation of total deformation by incorporating the phenomenological creep model of Shyam Sunder and Wu (1990). The stress-strain curves predicted from the model fit the experimental data reasonably well. The incorporation of the grain boundary dislocation mechanism and the creep model increase the strain and the compliance.

5.1 Introduction
The ductile-to-brittle transition is important in engineering application because the maximum compressive strength and thus the maximum ice load against a offshore structure occurs in this region. Ice becomes either ductile or brittle depending on the loading conditions. Schulson (1990) shows that ice is generally ductile under the loading rates lower than $10^{-4}s^{-1}$ and the stress-strain curve is characterized by the peak between the ascending and descending branch. When the strain rates go beyond approximately $10^{-3}s^{-1}$, the ice becomes brittle and the stress-strain curve has only ascending branch. The strain rate that marks the transition increases as the grain size decreases and the lateral confinement increases (Cole, 1985).

The deformation behavior of polycrystalline ice in the ductile-brittle transition is characterized by: (i) crack nucleation and progressive damage; and (ii) transient creep. The former contributes to the increase of compliance and the final failure, and the latter causes large strain. The nucleation of the first crack generally govern the failure stress in tensile tests. Under compression, however, the microcracks get arrested shortly after nucleation and the progressive nucleation of microcracks contributes to the accumulation of damage.

It is generally agreed that the crack nucleation in ice is caused by the stress concentrations resulting from dislocation pileup and elastic anisotropy mechanism. The dislocation pileup mechanism is observed below the transition domain where ice shows ductile behavior, whereas the elastic anisotropy mechanism is considered to be dominant above the transition domain.

Gold (1972), from the statistical analysis of the observations on the strain dependence of the crack density, found that there can be two independent families of cracks; the one dependent on the creep strain, the other independent of it. He proposed that dislocation pileup is responsible for the first family of cracks, while the growth of nuclei due to diffusion or a local stress causes the second type of cracks.

Cole (1988) studied the dislocation pileup and the elastic anisotropy as underlying mechanisms for crack nucleation in polycrystalline ice. After assuming that there exist a
sufficient number of glissile dislocations at the start of straining he computed the time of
moving the existing dislocations into a pileup of specific length. According to the result the
time required for a dislocation to travel to the pileup position is several times higher than the
value for the first crack nucleation found in experiments. Based on the results it is
concluded that cracks nucleate due to (i) strain dependent dislocation pileup mechanism
when the strain rate is lower than the transition domain, and (ii) strain independent elastic
anisotropy mechanism under strain rate higher than the transition.

From the observation that cracks form in a time period too short for the pileup of
dislocations to cause significantly large stress concentrations at the high end of the ductile-
brittle transition, Shyam Sunder and Wu (1990) have studied the elastic anisotropy
mechanism as a main cause of the crack nucleation in polycrystalline ice. They postulated
that a precursor or a small starter crack exists as a result of the elastic property mismatch
between ice crystals. They also calculated microstructural stresses resulting from the elastic
anisotropy mechanism based on the first order approximation of the Eshelby (1957)
procedure, and included that in the computation of the nucleation stress and the evolution of
the elastic constants.

Wu and Niu (1995) formulated the grain boundary dislocation pileup mechanism to
model the formation of precursors. Their formulation is based on the X-ray topographical
observations of Hondoh and Higashi (1983) that the grain boundary dislocations are
generated from sources on grain boundaries and are accumulated to cause stress
concentrations. They concluded that the stress concentration due to the elastic anisotropy
mechanism and the grain boundary dislocation pileup at triple points are sufficient to cause
precursors at grain boundary triple points under small applied stresses. They also found
that unstable Griffith cracks are also possible at large applied stresses.

The precursor may grow along the grain boundary or into the crystals (Cole, 1985).
Canon et al. (1990), from compression tests of columnar ice, observed wing cracks
sprouted from inclined cracks which are located at the grain boundaries with approximate
length of boundary facets. Based on their findings, Elvin and Shyam Sunder (1994) developed a micromechanical damage model for polycrystalline ice in the high end of the ductile-brittle transition and brittle regime. They postulated that a precursor, which is pre-existing as a result of elastic property mismatch, first nucleates into a grain boundary crack, and then grows into neighboring crystals to form a wing crack.

In this study a damage model to predict the behavior of ice in the ductile-to-brittle transition will be presented. The model will include the dislocation pileup as well as the elastic anisotropy mechanism for crack nucleation, the formation of grain boundary cracks and subsequent growth into wing cracks, and the deformation by creep. The grain boundary dislocation pileup mechanism of Wu and Niu (1995) will be adopted for crack nucleation, and the approach of Elvin and Shyam Sunder (1994) will be followed to formulate the growth of the microcrack and to evaluate the increase of compliance due to damage. The effect of creep on the total deformation of ice will be considered by the phenomenological creep model of Shyam Sunder and Wu (1990). The possible interaction between creep and damage will not be considered in this model.

5.2 Modeling of damage

5.2.1 Microstructural Stresses

Because of the elastic property mismatch between grains, the differently oriented constituent crystals tend to deform incompatibly. Since this incompatibility is not realized, microstructural stresses are generated. The analysis of the microstructural stress is based on the first order approximation of the Eshelby (1957) procedure. Consider a grain boundary crack of length 2c with orientation β and grains around it with various c-axis orientations as shown in Fig. 5.1. If the grains surrounding the microcrack are separated,
the behavior of these grains can be defined in terms of the elastic stress-strain relations for single ice crystals, i.e.:

\[ \varepsilon_g = S_g \sigma_a \] (5.1)

where \( \sigma_a \) is the applied stress, \( \varepsilon_g \) and \( S_g \) are the strain and the compliance of a single crystal, respectively. The compliance matrix of a single ice crystal determined by Gammon et al. (1983) at temperature T=−16ºC are given as follows.

\[
[S_g] = \begin{bmatrix}
1.0318 & -0.2316 & -0.4287 \\
0.8441 & -0.2316 & 0 \\
1.0318 & 3.3179 & 2.9210 \\
\text{sym.} & 3.3179 & \\
\end{bmatrix} 10^{-1}\text{GPa}^{-1} \] (5.2)

where the plane of transverse isotropy is contained in the \( X_1-X_3 \) plane, and the \( c \)-axis is in the \( X_2 \) direction. The remaining matrix has the elastic property of isotropic polycrystal body, i.e.:

\[ \varepsilon = S \sigma_a \] (5.3)

where \( \varepsilon \) is the strain vector induced in the homogeneous matrix and \( S \) is the compliance tensor of the polycrystal. The elastic constants of polycrystalline ice are determined by the distribution of the crystallographic orientation of each grain. The undamaged compliance matrix of isotropic granular ice at -16ºC are (Gammon et al. (1983)):
\[
[S] = \begin{bmatrix}
1.0716 & -0.3486 & -0.3486 \\
1.0716 & -0.3486 & 0 \\
1.0716 & 2.8401 & \text{sym} \\
\end{bmatrix}
\]

\[10^{-1}\text{GPa}^{-1} \quad (5.4)\]

The corresponding stiffness matrices can be obtained by inverting the compliance matrices. The above 3-D matrices can be transformed into plane strain matrices using the relation given by Savin (1961). The transformed plain strain components of the compliance matrix of the single and polycrystalline ice become:

\[
[S_e] = \begin{bmatrix}
0.8537 & -0.3278 & 0 \\
0.7921 & 0 & \text{sym} \\
\end{bmatrix} \quad 10^{-1}\text{GPa}^{-1} 
\]

\[(5.5)\]

\[
[S] = \begin{bmatrix}
0.9582 & -0.4620 & 0 \\
0.9582 & 0 & \text{sym} \\
\end{bmatrix} \quad 10^{-1}\text{GPa}^{-1} 
\]

\[(5.6)\]

When the body is already damaged with cracks, \(S\) should be replaced by the effective (damaged) solid compliance matrix.

Once the separated grains are fitted back to the polycrystal matrix, microstructural stresses are induced in the grain due to the misfit between matrix strain and the strain of the crystal allowed to deform freely:

\[
\sigma_o = \frac{1}{2} \left[ [C_g(\zeta_1) + C_g(\zeta_2)]S - 2I \right] \sigma_s 
\]

\[(5.7)\]
where $C_g$ is the elastic stiffness of single ice crystal dependent on the basal plain orientation $\zeta$. Under uniaxial compression the induced microstructural stresses due to elastic anisotropy in ice can be as large as 20% of the applied stress, and they may be tensile or compressive depending on the crystallographic orientations of the grains. The nominal applied stress will be enhanced as microcracks nucleate in the material. Consequently, the total stress results in:

$$\sigma = \sigma_0(\zeta) + \sigma_a$$  \hspace{1cm} (5.8)

The total stress obtained above is used in the computation of the evolution of compliance and total strain.

5.2.2 Nucleation of microcracks

In the formulation of the grain boundary dislocation pileup mechanism of Wu and Niu (1994), it is assumed that the pileup groups are similar to the pileups of lattice dislocations against the grain boundaries as formulated by Eshelby et al. (1953). Fig. 5.2 shows the schematic of grain boundary dislocation pileup at a triple point. The contributions of the three pileup groups are combined vectorially as the grain boundary dislocations enter the crack. The microstructural stresses are independently added to the remote shear stress acting on the grain boundaries. In this paper it is assumed that the ice crystals are regular hexagons so that the angles between the grain boundaries are $2\pi/3$. Also the grain boundary and basal plane orientations are assumed to be uniformly distributed from zero to $\pi$.

Due to the interactions between grain boundaries, the resultant distribution of shear stresses on the grain boundaries are initially unknown. The influence shear stress on the
The influence stress at the ith boundary due to an average effective shear stress on jth boundary is given by (Stroh, 1954):

$$
\tau_{ij} = \tau_j \left( \frac{l_j}{x_i} \right)^{1/2} \cos \frac{\theta_{ij}}{2} \left[ 1 - 3\sin^2 \frac{\theta_{ij}}{2} \right]
$$

(5.9)

where \( \tau_j \) is the initially unknown effective stress on jth boundary, \( l_j \) is the length of the dislocation pileup, \( x_i \) is the coordinate measured from the triple point, and \( \theta_{ij} \) is the orientation of boundary i relative to boundary j. The average influence shear stress is obtained after the integration:

$$
\frac{1}{n_i} \int_0^{l_i} \rho_i \tau_j \, dx_i = \alpha_j \tau_j \quad \text{(no summation)}
$$

(5.10)

where \( n_i \) is the number of dislocations in the ith boundary, \( r_o \) is of the order of dislocation core radius, and \( \rho_i \) is the density distribution function on the ith boundary given by Eshelby et al. (1953):

$$
\rho_i = \frac{2n_i}{\pi l_i} \left( \frac{l_i - x_i}{x_i} \right)^{1/2}
$$

(5.11)

These influence shear stresses from the other two boundaries are added to the shear stress resulting from both remote stress and microstructural stress to give the effective shear stress \( \tau_i \).

After the effective shear stresses on all grain boundaries are obtained, the ledge strength \( B_i \) on the ith grain boundary is given by:

$$
B_i = \pi \frac{1 - v}{G} |\tau_i| \eta L_i
$$

(5.12)
where \( \nu \) is the Poisson's ratio, \( \eta \) is a constant representing the distance between the triple point and the nearest dislocation source and \( L_i \) is the grain boundary facet length.

Using the above relations the energy of the crack system \( W \) and the energy of dislocation pileup groups \( W_{gr} \) result in (Wu and Niu, 1994):

\[
W = 2yC + \left( \frac{1}{4\pi(1-\nu)} \ln \frac{4R}{b} - \frac{1}{4\pi(1-\nu)} \ln \frac{c}{b} \right) \\
-\frac{\pi(1-\nu)}{8G} [c^2 + (\sigma_n^2 + (\sigma_p^2)] c^2 - \frac{\sigma_n B_n + \sigma_p B_p}{2} c
\]

\[
W_{gr} = \frac{G}{4\pi(1-\nu)} \sum_{i=1}^{3} B_i^2 \left[ \ln \frac{4\pi e^{1/2} (1-\nu) \tau_i l_i R}{B_i G} - \frac{1}{n_i} \ln \frac{4\pi (1-\nu) \tau_i l_i}{b G} - \frac{1}{6n_i^2} \ln n_i \right]
\]

(5.13)

(5.14)

where \( \sigma_n \) and \( \sigma_p \) are the total normal and shear stresses acting on the crack, respectively, and \( B_n \) and \( B_p \) are sum of the normal and shear components of ledge strength, respectively.

The stresses are sum of the remote stress and the microstructural stress. In the original formulation of Wu and Niu (1995) the complete Eshelby method was used for the microstructural stress, whereas the first-order approximation is made in this research.

The microcrack is assumed to nucleate if the energy of the pileup group is greater than the energy of the crack system:

\[
\Delta W = W_{gr} - W > 0
\]

(5.15)

The length of the microcrack can be obtained by equating the derivative of the energy of crack system with respect to the crack length to zero, and the crack remains stable if the second derivative of the energy of the crack system is positive, and is unstable if the second derivative results in negative value. Wu and Niu (1995) shows that the stable precursor
nucleation is possible at the triple points, depending on the dislocation state and loading condition. They also shows that the predicted precursor lengths do not differ significantly between tension and compression at small applied stresses. The shortest stable precursor is as small as 1% of the grain facet length, whereas it can be as long as about 10% of the facet under compression. When the nucleated precursors turn out to be unstable, they are set to directly form grain boundary cracks. As the small stable cracks do not contribute much to the increase of compliance, only the grain boundary cracks are considered in the computation of the stress-strain relation.

5.2.3 Formation of wing cracks

The frictional sliding of the grain boundary crack produces tension crack at the tips of the grain boundary crack, which grows in the direction of maximum compression. This phenomenon has been observed in ice by Canon et al. (1990). Elvin and Shyam Sunder (1995) formulated the evolution of damage due to the wing crack formation in ice based on the approximate approach of Horii and Nemat-Nasser (1986), where the wing crack is replaced by a straight crack with point force at the middle of the crack. The point force results from the sliding of the grain boundary crack. Horii and Nemat-Nasser (1986) shows that the stress intensity factors obtained from the approximate method are reasonably close to the exact solution computed from singular integral equations and numerical analysis.

The component of the normal and shear stress acting on the grain boundary cracks are determined from the components in the global frame by:

\[
\sigma'_{11} = \left(\sigma_{22} + \sigma_{11}\right)/2 + \left[\left(\sigma_{22} - \sigma_{11}\right)/2\right]\cos2\beta - \sigma_{12}\sin2\beta
\]

\[
\sigma'_{12} = -\left[\left(\sigma_{22} - \sigma_{11}\right)/2\right]\sin2\beta - \sigma_{12}\cos2\beta \pm \mu\sigma'_{11}
\]  

(5.16)
where $\mu$ is the coefficient of friction, $\beta$ is the grain boundary orientation which is the same with the precursor orientation, and $\mu \sigma_{11}'$ is the Coulombic frictional stress which opposes sliding when the normal stress is compressive. The effective shear stress $\sigma_{12}'$ is set to zero when the magnitude of the total shear stress acting on the crack is smaller than or equal to that of the frictional stress. The wing crack is formed when the stress field around the grain boundary crack satisfies the maximum principal tensile stress criterion of Erdogan and Sih (1963):

$$K_1 \cos^3 \frac{\theta_m}{2} - 3K_\Pi \cos^2 \frac{\theta_m}{2} \sin \frac{\theta_m}{2} = k_{iC}$$

(5.17)

where $\theta_m$ is given by:

$$\tan \frac{\theta_m}{2} = \frac{1}{4} \left[ \frac{K_1}{K_\Pi} \pm \sqrt{\left( \frac{K_1}{K_\Pi} \right)^2 + 8} \right]$$

(5.18)

The mode I and II stress intensity factors become:

$$K_1 = \sigma_{11}' \sqrt{\pi h}$$

$$K_\Pi = \sigma_{12}' \sqrt{\pi h}$$

(5.19)

where $h$ is the half length of the grain boundary crack. If the normal stress is compressive, it is assumed that the crack is closed and consequently $K_1=0$. The macrostructural fracture toughness $K_{iC}$ can be obtained from experimental data (Nixon and Schulson, 1987).
Once the wing crack is formed, it is replaced by the representative straight crack with a point force in the middle (Fig. 5.3). The point force $F$ is obtained by:

$$F = 2h\sigma'_{12}$$  \hspace{1cm} (5.20)

With the point load the mode I and II stress intensity factor of the representative straight crack are given by (Horii and Nemat-Nasser, 1986):

$$K_I = \sigma_{11}' \sqrt{\pi c} + \frac{F \sin \theta}{\sqrt{\pi (c + c')}}$$  \hspace{1cm} (5.21)

$$K_{II} = \sigma_{22}' \sqrt{\pi c} + \frac{F \cos \theta}{\sqrt{\pi (c + c')}}$$  \hspace{1cm} (5.22)

where $\theta = \beta - \gamma$, $c$ is the half length of the representative straight crack, and $c'$ is the correction factor with the value of 0.27 times the facet length needed to insure that the stress-intensity factor are bounded at the initiation of the wing cracks (Horii and Nemat-Nasser, 1986). The wing cracks are assumed to grow when the mode I stress intensity factor exceeds the macroscopic fracture toughness $K_{IC}$. The length of the straight crack is determined by equating $K_I$ to $K_{IC}$, and the orientation is obtained from maximizing $K_I$ with respect to $\theta$. This approach is proved to be a good approximation of the exact numerical solutions (Horii and Nemat-Nasser, 1986). Fig. 5.3 shows the schematic of wing crack formation from a grain boundary crack, and the approximation into a straight crack with point force.

When the grain boundary crack is subjected to tensile stress normal to its length, it will sprout wing crack which propagates unstably through the neighboring crystals. On the other hand, if the stress field is compressive and the crack slides, the wing crack can be either stable or unstable depending on the stress states. Elvin and Shyam Sunder (1995)
shows that the wing cracks grow stably under biaxial compression, but under tensile lateral stress the wing crack propagates unstably. In this study the wing crack is assumed to be arrested at the neighboring grain boundaries and consequently the maximum length of the representative straight crack is $2d$, where $d$ is the grain size. Further propagation of the arrested cracks leading to final failure will not be considered in this study. After the wing crack is formed only the applied stress will be applied in the analysis since the first-order approximation of the microstructural stress may not be accurate for the cracks longer than the size of grains.

5.2.4 Elastic compliance of a damaged ice

The damaged compliance $S$ can be divided into the original compliance $S_0$ and the additional compliance $H$ generated from the nucleation of the microcracks:

$$S = S_0 + H$$  \hspace{1cm} (5.23)

$H$ can be expressed as following when the crack length and the grain size are constant, and the orientations of the precursor and the basal plane are uniformly distributed from 0 to $\pi$:

$$H_{ij} = \frac{M}{\pi^2} \int (K_{ki}^g + K_{ki}^w) T_{ki} T_{ij} \, d\zeta \, d\beta$$  \hspace{1cm} (5.24)

where $M = 12 / \pi d^2$ represents the maximum number of precursors per unit area in the given stress assuming that there are maximum number of 2 precursors per grain and the number of microcracks per grain is $6 / \pi d^2$ (Cole, 1986). $K^g$ is the contribution of the single grain boundary crack to the additional compliance, and $K^w$ is the contribution of a wing crack. They are obtained from crack opening displacement and the derivation can be found in Elvin and Shyam Sunder (1995).
5.2.5 Computation of creep strain

In brittle ice the strain at failure predicted by a elastic damage model of Kim et. al. (1995) underestimates the maximum strain obtained from experiments (Cole, 1985). In the ductile-brittle transition the creep strain contributes to a large proportion of the total deformation of polycrystalline ice. In this paper, the physically-based internal variable creep model of Shyam Sunder and Wu (1989) is used to compute the creep strain. For simplicity, it is assumed that there exists no physical coupling between the mechanisms of creep and elastic damage.

In this creep model the total strain rate is additively decomposed as follows:

$$\dot{\epsilon} = \dot{\epsilon}_e + \dot{\epsilon}_v + \dot{\epsilon}_t$$  \hspace{1cm} (5.25)

where the subscript $e,v$ and $t$ denote the elastic, viscous and transient components of the strain rate, respectively.

The viscous strain rate vector $\dot{\epsilon}_v$ is represented by the classical power law:

$$\dot{\epsilon}_v = \dot{\epsilon}_0 \lambda G \sigma$$

$$\lambda = \frac{3}{\beta} \left[ \frac{L}{V} \right]^N \sigma_{eq}^{N-1}$$  \hspace{1cm} (5.26)

where $\dot{\epsilon}_0$ is the reference strain rate, $G$ is the matrix which transforms stresses into deviatoric components, $\beta$ is the parameter representing fabric anisotropy, $N$ is the power law exponent, $\sigma_{eq}$ is the equivalent stress, and $V$ is the temperature-dependent creep resistance. The transformation matrix $G$ is given by:
\[
G = \begin{bmatrix}
\frac{a_1 + a_3}{3} & \frac{-a_1}{3} & \frac{-a_3}{3} \\
\frac{a_1 + a_3}{3} & \frac{-a_2}{3} & 0 \\
\frac{a_1 + a_3}{3} & \frac{2a_4}{3} & 2a_5 \\
sym. & 2a_6
\end{bmatrix}
\] (5.27)

The orthotropic parameters \(a_1 - a_6\) can be estimated from experimental data under steady flow conditions (see Ting and Shyam Sunder, 1985, for details). For an isotropic material the parameters are equal to unity.

Transient creep in ice is fully recoverable upon unloading while viscous creep is irrecoverable. The transient strain rate is given by:

\[
\dot{\epsilon}_t = \dot{\epsilon}_0 \lambda_d G(\sigma - R) \quad \lambda_d = \frac{3}{\beta} \left[ \frac{I}{BV} \right]^N \sigma_{r,eq}^{N-1}
\] (5.28)

where \(\sigma - R\) is the reduced stress and \(\sigma_{r,eq}\) is the equivalent measure of the reduced stress.

\(R\) is a second-rank tensor which represents the internal stress associated with the complex interactions between the soft and hard deformation system, \(B\) is a scalar representing the isotropic hardening associated with the interaction of dislocations. The evolutions of the internal state variable \(R\) and \(B\) are expressed by:

\[
\dot{R} = \frac{\beta}{3} AEH \dot{\epsilon}_t
\] (5.29)

\[
\dot{B} = \Theta \left[ \frac{\tilde{H}E}{\sigma_{d,eq}} \right] \dot{\epsilon}_{t,eq}
\] (5.30)
where $A$ is a non-dimensional constant to represent the anelasticity of a material, $H$ is a matrix which transforms the strains into their deviatoric components, $\dot{H}$ is the material constant which describes the rate of isotropic hardening, and $\Theta$ makes $B$ approach the threshold value $B_0$ asymptotically in case of unloading. The transformation matrix $H$ is given by:

$$
H = \begin{bmatrix}
\frac{3(a_1 + a_3)}{a^2} a_2^2 & -\frac{3a_1 a_2 a_3}{a^2} & -\frac{3a_1 a_2 a_3}{a^2} \\
\frac{3(a_2 + a_3)}{a^2} a_1^2 & \frac{3a_1 a_2 a_3}{a^2} & 0 \\
\frac{3(a_1 + a_2)}{a^2} a_3^2 & \frac{1}{2a_4} & \frac{1}{2a_5} \\
\text{sym.} & \frac{1}{2a_6} & 1
\end{bmatrix} \quad (5.31)
$$

Readers are referred to Shyam Sunder and Wu (1990a) for the physical basis of the constitutive model and its material parameters.

5.3 Numerical results

5.3.1 Model parameters

For the transversely isotropic polycrystalline ice under plane strain condition, the Young's modulus $E$ is 9.369 GPa, the shear modulus $G$ is 3.535 GPa, and the Poison ratio is 0.325. The surface energy $\gamma$ is taken to be 0.0765 J/m2 from Ketcham and Hobbs (1969).
The friction stress $\tau_f$ for dislocation glide along the grain boundary is taken to be 0.1 MPa considering the observation by Hondoh and Higashi (1983). The Burgers vector $b$ is assumed to be $0.6a$ following the approach of Wu and Niu (1995) where $a = 4.52 \times 10^{-10} m$ is the lattice parameter of ice. The parameter $\eta$ which determines the number of the grain boundary dislocations is taken to be 0.15 (Wu and Niu, 1995).

Furthermore the grain boundary facet length $L$ is taken to be $0.55d$ assuming a regular hexagon, where $d$ is the grain size. The macroscopic fracture toughness varies from about 0.08 to 0.12 MPam$^{0.5}$ depending on the change in temperature (Nixon and Schulson, 1987). The friction coefficient between crack surfaces is function of strain rate and temperature (Schulson, 1990). In ductile-brittle transition the value is within 0.4-0.6.

The parameters for the creep model have been estimated from uniaxial compressive creep tests on polycrystalline ice (Shyam Sunder and Wu, 1989). The parameters used in this study are obtained from constant-stress creep tests on isotropic polycrystalline ice. Table 5.1 shows the values of model parameter obtained from the experimental data of Jacka(1984). The value of the activation energy, $Q$, has been estimated to be about 67 KJmol$^{-1}$ (Gold, 1973).

5.3.2 Model prediction of stress-strain curve

In this study the constitutive relation of polycrystalline ice in ductile-to-brittle transition regime is predicted using the micromechanical model described in the previous section. The maximum strains at failure predicted by the microstructural model of Shyam Sunder et. al. (1995) underestimate the experimental data because it does not include: (i) effect of creep, (ii) crack nucleation due to dislocation pile-up mechanism, and (iii) formation of wing cracks. The consideration of those mechanisms are required for ice in the lower end of the ductile-to-brittle transition.
Fig. 5.4 compares the stress for the first crack nucleation predicted from the elastic anisotropy mechanism and the dislocation pile-up mechanism. According to the results the dislocation pile-up mechanism predicts the microcrack nucleation in an earlier stage.

Fig. 5.5 shows the evolution of the compliance simulated from the models formulated with the dislocation pile-up mechanism and the elastic anisotropy mechanism. From the results it can be observed that the compliances computed from the dislocation pile-up mechanism grows faster than those predicted by the elastic anisotropy mechanism. This is due to the fact that (i) the dislocation pile-up mechanism predicts the nucleation of microcracks in an earlier stage, (ii) more damage is predicted from the model. The difference is more pronounced in the shear compliance.

Fig. 5.6(a) and 5.6(b) compare the stress-strain relations of granular ice with and without considering the above mechanisms. In Fig. 5.6(a) the predicted stress-strain curve for ice with grain size of 1.1 mm are compared with the experimental data of Schulson (1990) obtained at T=−10°C at the strain rate of 10⁻³s⁻¹. For the simulation the friction coefficient of 0.5 is used based on the experimental observation (Schulson, 1990), and the macroscopic fracture toughness of 80 KPam⁰.⁵ is taken from the experiments of Nixon and Schulson (1987). Similarly the model predictions of stress and strain relation for granular ice with mean grain size of 5.5 mm obtained under the same conditions are shown in Fig. 5.6(b). From the figures it can be found that the stress-strain curve obtained from the model including both the creep and dislocation pileup mechanisms overestimates the experimental data at high stress, whereas the results from the model with only the dislocation pileup mechanism underestimates the experimental data. The model with only the elastic anisotropy mechanism produces the smallest strain. Fig. 5.7(a) and 5.7(b) show the model predictions of the stress-strain curve and the experimental data of Cole (1985) obtained at the strain rates of 10⁻⁴s⁻¹ and 10⁻⁵s⁻¹, respectively. In these strain rates, which correspond to the mid- and low-end of the ductile-brittle transition, the model predictions considering all the mechanisms form a lower bound of the experimental data.
The results imply that there can be more mechanisms acting on the deformation of ice in this regime than considered in this study. In addition, the model lacks the mechanism for predicting the peaks and the descending branches in the stress-strain relation. This phenomenon is considered to be due to the interaction of cracks or due to the effect of tertiary creep. These effects are not considered in this study. Below the strain rate of about $10^{-6}\text{s}^{-1}$, there is a mechanism causing deformation even when there is no visible cracks. From compressive tests on various sizes of polycrystalline ice, Cole (1983) found that fine-grained ice exhibits no internal cracking at strain-rates below approximately $10^{-6}\text{s}^{-1}$ at $-5^\circ\text{C}$. Based on the results, he concluded that the material below the threshold for internal cracking is characterized by strain-induced boundary migration. It is also observed that at the low strain rate tests of fine-grained specimen the grain sizes are enlarged as a results of dynamic recrystallization. Dynamic recrystallization, and the strain-induced boundary migration in particular, is considered to be the cause for the onset of tertiary creep in ice when there is no significant internal cracking (Cole, 1987).

5.4 Conclusion

In this research the behavior of ice subjected to a strain rate in the ductile-brittle transition is simulated using a micromechanical model. The mechanisms of dislocation pile-up and the elastic anisotropy are considered in microcrack nucleation. The microcracks are assumed to initiate at triple points and grow along the grain boundary until they are arrested at neighboring triple points. The grain boundary cracks extend into the neighboring crystals when the wedging forces resulting from sliding of the grain boundary cracks satisfy the maximum tensile principal stress fracture criterion. The evolution of the compliance is computed considering the damage caused by the grain boundary cracks and wing cracks. The physically based phenomenological creep model developed by Shyam Sunder and Wu (1990) is combined with the damage model to obtain a more general
constitutive model for ice. In this research it is assumed that the damage process (i.e., evolution of elastic moduli) is not affected by the macroscopic creep deformation.

According to the results, the stress for the first nucleation of a microcrack predicted by the dislocation pile-up mechanism is much lower than the corresponding value obtained by the elastic anisotropy mechanism. The predicted stress-strain curves are generally in good agreements with the experimental data obtained at the strain rate in the ductile-brittle transition. However it still remains to be studied how to model the peak and the descending branch of the stress-strain curve in this region.
References


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Gold, L. W. (1972), The process of failure in columnar-grained ice, *Philosophical Magazine*, 26, 311-328


Table 5.1 Parameters for creep model (from Shyam Sunder and Wu, 1989)

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values determined from Jacka (1984)</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td>9.5 GPa</td>
</tr>
<tr>
<td>N</td>
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</tr>
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<tr>
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Fig. 5.1 The coordinate system and the basal plane orientations.
Fig. 5.2 Schematic of grain boundary dislocation pile-up at a triple point.
Fig. 5.3 Approximation of wing crack with a representative straight crack with point force.
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CHAPTER VI

MICROMECHANICAL MODEL FOR THE CONSTITUTIVE RELATION OF CONCRETE

Abstract

In this study the stress-strain relation of a plane concrete will be predicted using a micromechanical model. The precursor is assumed to exist in the aggregate-hardened cement paste interface. The pre-existing defects form during hydration process, mainly by bleeding and the non-homogeneity in elastic property of the constituent materials. When a fracture criterion is satisfied the pre-existing defects nucleate into bond cracks along the interfaces which have smallest fracture toughness. Once the bond cracks are formed they grow into mortar as the loading increases. Under tensile loading the wing crack is assumed to propagate unstably through the specimen as soon as it nucleates. Under compression, however, the wing crack grows in a stable manner until it becomes unstable. In this study it is assumed that the unstable propagation of wing crack stops at the neighboring aggregates under compression, whereas it causes unstable failure under tension. The overall compliance is calculated from the damage due to microcracks, and the predicted stress-strain curves are compared with experimental data. According to the parametric studies, the predicted strain increases as the volume fraction and size of the aggregates increase. The model predictions turn out to be in reasonable agreement with the experimental data.

6.1 Introduction

Concrete is a porous composite material consisting mainly of hardened cement paste, aggregates and water. Three levels of modeling of concrete structure are generally
used (Wittman, 1983): On the micro-level, concrete consists of crystals of calcium silicate hydrate with primary and secondary bonds. The meso-level considers the composite nature of concrete and distinguishes between hardened cement pastes, aggregate, and a bond layer between these three constituents. On the macro-level, concrete is modeled as a homogeneous isotropic material containing flaws.

The stress-strain curve for aggregate in compression is essentially linear to the point of failure, and the curve for the cement paste is linear up to 90 to 95% of its strength. However, the stress-strain relation for concrete is highly non-linear. This nonlinearity is due not only to the composite action of the material, but also to the nature of the cement-aggregate bond. It is observed that a reduction in bond strength leads to an increase in the nonlinearity of the stress-strain curves, and stronger concretes exhibit a more linear stress-strain curve.

Before loading there exists a highly imperfect bond between the aggregate and the hardened cement paste. These are due to: (i) bleeding beneath aggregates, (ii) incompatibility in the elastic moduli of the hardened cement and the aggregate, which leads to stress concentrations under the differential volume changes due to continued hydration and drying of the cement, (iii) different thermal expansion property, and (iv) different response to moisture content.

Brittle materials tend to develop tensile cracks perpendicular to the direction of the largest tensile strain. Thus when concrete is subjected to uniaxial compression, cracks occur parallel to the maximum compressive stress, and this process results in redistribution of internal stress and thus the deviation of the stress-strain curve from the linear line (Mindess, 1983). It is observed that cracks go around the aggregates in normal concrete whereas in high-strength concrete some cracks go through the aggregates. Fig. 6.1 shows the schematic of the location and growth of cracks in concrete.

As loading increases, a considerable amount of progressive cracking takes place. Microcracks that occur along the interface between paste and aggregate are called bond
cracks, and those that cross the mortar are known as mortar cracks. Generally the length of microcracks varies depending on the size of aggregates, water-cement ratio and mix-proportion, etc.

Experimental observations show that there are four major stages in the development of microcracking and failure in concrete subjected to uniaxial compressive loading (Macgregor, 1988):

1. The pre-existing cracks have little effect on the integrity of the concrete at low loads and the stress-strain curve remains linear up to about 30% of the compressive strength of the concrete.

2. When concrete is subjected to short-term stresses greater than 30 to 40% of the strength, the combination of stresses on the inclined surfaces of the aggregate particles will exceed the tensile and shear strengths of the paste-aggregate interfaces and bond cracks will develop. These cracks are stable and propagate only if the load is increased. Once such a crack has formed, however, any additional load that would have been transformed across the cracked interface is redistributed to the remaining unbroken interfaces and mortar.

3. As the load is increased beyond 50 or 60% of ultimate, localized mortar cracks develop, which grow parallel to the direction of the compressive loading. During this stage, there is stable crack propagation; cracking increases with increasing load but does not increase under constant load.

4. At 75 to 80% of the ultimate load, the number of mortar cracks begins to increase and a continuous pattern of microcracks begins to form. Eventually, the load-carrying capacity of the uncracked portions of the concrete reaches a maximum value regarded to as the compressive strength. Further straining is accompanied by a drop in the stress that the concrete can resist.

Under uniaxial tension the stress-strain diagram is linear up to about 80% of the failure stress (Ziegeldorf, 1983). The deviation of the stress-strain curve from linear line is linked to the nucleation of the bond cracks. As the external load is increased some of the
bond cracks grow into the paste, and as soon as the microcracks are connected to form a continuous crack, peak load is reached.

The tensile failure of concrete is characterized by the failure surface perpendicular to the direction of the tensile loading, whereas under uniaxial compression the failure surface is vertical when frictionless load bearing platens are used, and is inclined when rigid platens are used, which inflict confinement at the loading surfaces. For higher strength concrete the stress-strain curve is steeper and linear up to a higher stress-strength ratio than in normal concrete because the over-all bond cracking is decreased. In this case the failure surface is smoother and more vertical (Ziegeldorf, 1983).

There have been diverse approaches to model the macroscopic response of concrete under multiple loading conditions. The phenomenological models based on plasticity theory does not implement the microstructural damage process, whereas the continuum damage models frequently use arbitrarily chosen equations and parameters to describe the microcrack growth and damage evolution.

The micromechanical model predicts the brittle deformation process of a quasi-brittle material with the formation and growth of internal cracks, taking into account only the physically explainable parameters. Kachanov (1982) and Nemat-Nasser and Obata (1988) proposed a micromechanical damage model for rock, and Fanella and Krajcinovic (1988) and Fanella (1990) for concrete, and Wu and Shyam Sunder (1992) for polycrystalline ice.

Generally the micromechanical damage models of concrete and other brittle materials are based on fracture mechanics to describe the internal cracking phenomenon and the progressive damage process. With the linear elastic fracture mechanics it is often possible to find a general analytical solutions, which are easier to handle than the numerical analysis using finite element method. However the fracture process of concrete structure deviates from linear elastic fracture mechanics due to the development of a relatively large fracture process zone composed of accumulation of microcracks in front of a major crack.
(Hillerborg, 1983). However it may be reasonable to use LEFM to examine the fracture of unnotched concrete specimens if its microscopic structure is considered (Wang, et al., 1993).

In this study the micromechanical damage model based on the work of Horii and Nemat-Nasser (1983, 1986) will be applied to predict the constitutive relation of plane concrete under the loading that causes brittle behavior in the material. It is assumed that the constituent materials are elastic. The cement-aggregate composite is replaced by a homogeneous elastic material with a set of imaginary interface boundaries. The linear elastic fracture mechanics will be applied to predict the nucleation and growth of cracks under uniaxial and biaxial loading. The tensile failure stress will be predicted from the fundamental argument of LEFM. The effect of creep or shrinkage will be neglected as the short-term loading is considered in this research.

6.2 Micromechanical model

6.2.1 Formation of initial defects

As mentioned above, the initial defects (no-load bond cracks) are caused by bleeding, shrinkage, cement hydration heat, etc., and are concentrated at the cement paste-aggregate interfaces. It is assumed that the initial defects, which we call precursors, are randomly distributed and their size are proportional to the size of the aggregates. These cracks do not affect the strength of the material until the loading reaches a certain magnitude that nucleates the precursors into bond cracks with the length of the aggregate facet. In this study the length of the precursor is taken to be proportional to the length of the aggregate facet. Similar approach has been taken by Krajcinovic and Fanella (1986). Fig. 6.1(a) shows a coarse aggregate and the location of a initial defect.
6.2.2 Nucleation of bond-cracks

The microstructure of concrete is not homogeneous due to existence of aggregates, as are the stress and strain fields. The macroscopic values of the stress and strain used in this analysis are actually representative values which can be expressed as the average of the local values over the area:

\[ \sigma = \frac{1}{A} \int \bar{\sigma} \, dA \]  

(6.1)

\[ \varepsilon = \frac{1}{A} \int \bar{\varepsilon} \, dA \]  

(6.2)

As the aggregates are randomly distributed, it is reasonable to assume that the material is elastic, homogeneous and isotropic. Consider the precursor (initial defect) which is oriented at an angle \( \beta \) with the \( x_1 \) axis (Fig. 6.2) and is subjected to the remote normal stress \( \sigma'_{11} \) and shear stress \( \sigma'_{12} \) defined in a local coordinate \( x_1' - x_2' \):

\[
\sigma'_{11} = \left( \sigma_{22} + \sigma_{11} \right)/2 + \left[ \left( \sigma_{22} - \sigma_{11} \right)/2 \right] \cos 2\beta - \sigma_{12} \sin 2\beta
\]

\[
\sigma'_{12} = -\left[ \left( \sigma_{22} - \sigma_{11} \right)/2 \right] \sin 2\beta - \sigma_{12} \cos 2\beta \pm \mu \sigma'_{11}
\]  

(6.3)

where \( \mu \) is the coefficient of friction and \( \mu \sigma'_{11} \) is the Coulombic frictional stress which oppose sliding when the normal stress is compressive. The effective shear stress \( \sigma'_{12} \) is set to zero when the applied stress is smaller than or equal to the frictional stress. The mode I and II stress intensity factors become:

\[ K_1 = \sigma'_{11} \sqrt{\pi a} \]
\[ K_{II} = \sigma'_{12} \sqrt{\pi a} \]  

(6.4)

where \( a \) is the half precursor length. If the normal stress is compressive, it is assumed that the crack is closed and consequently \( K_1 = 0 \). The asymptotic distribution of the tangential and shear stresses can be expressed as follows:

\[ \sigma_{\theta\theta} = \frac{1}{\sqrt{2\pi r}} \cos \frac{\theta}{2} \left[ K_1 \cos^2 \frac{\theta}{2} - \frac{3}{2} K_\Pi \sin \theta \right] \]  

(6.5)

\[ \sigma_{r\theta} = \frac{1}{2\sqrt{2\pi r}} \cos \frac{\theta}{2} \left[ K_1 \sin \theta + K_{II} (\cos \theta - 1) \right] \]  

(6.6)

where \( r \) is the radial distance from the tip of the precursor and \( \theta \) is the angle measured anti-clockwise from a line extending along the precursor in the solid.

According to the maximum principal tensile stress criterion of Erdogan and Sih (1963), a precursor extends into a bond crack when the maximum value of the principal tensile stress given by the above equation has the same value as that for growth in an equivalent mode I problem, i.e. \( k_{IC}/(2\pi r)^{1/2} \). The growth condition is obtained by equating Eq. 6.5 with this quantity, i.e.:

\[ K_1 \cos^3 \frac{\theta_m}{2} - 3K_{II} \cos^2 \frac{\theta_m}{2} \sin \frac{\theta_m}{2} = k_{IC} \]  

(6.7)

where \( k_{IC} \) is the mode I fracture toughness of the cement paste-aggregate interface, and \( \theta_m \) is obtained by setting the \( \sigma_{r\theta} \) in Eq. 6.6 equal to zero, which is given by:

\[ \tan \frac{\theta_m}{2} = \frac{1}{4} \left[ \frac{K_1}{K_{II}} \pm \sqrt{\left( \frac{K_1}{K_{II}} \right)^2 + 8} \right] \]  

(6.8)
Eq. 6.8 yields two critical initial angles and the angle that yields the most positive value is chosen and compared with $k_{IC}$. Eq. 6.7 represents the kinetic law of bond crack formation, and as the applied stress is increased more and more precursors will nucleate into bond cracks. It is assumed that the precursor extends along the aggregate boundary and stops growing when it encounters the paste because the fracture toughness of cement paste is greater than that of interface (Zaitsev, 1983).

6.2.3 Formation of mortar cracks

Once a bond crack is formed along the aggregate boundary, it can be extended to out-of-crack-plane when a certain loading is reached (Zeitsev, 1983). The mixed mode stress field produces tension cracks at the tips of the bond crack, which subsequently grow into the mortar to form a mortar crack (Fig. 6.1). In Horii and Nemat-Nasser (1986), the bond crack-mortar crack combination is replaced by a straight crack with point force in the middle of the crack. The point force results from the sliding of the bond crack. Fig. 6.1(c) and 6.1(d) show the schematic of the mortar crack formation from a grain boundary crack, and the approximation into a straight crack with point force. Horii and Nemat-Nasser (1986) shows that the stress intensity factors obtained from the approximate method are reasonably close to the exact solution computed from singular integral equations and numerical analysis. The component of the normal and shear stress acting on the bond cracks are determined from the components in the global frame by Eq. 6.3. In this case $\beta$ is the bond crack orientation which is identical with the precursor orientation. For wing crack formation, the maximum principal tensile stress criterion in Eq. 6.7 is used again, but the fracture toughness of cement paste $K_{IC}$ is used in this case.
Once the wing crack is formed, the bond crack-wing crack combination is replaced by the representative straight crack with point force in the middle. The point force $F$ acting on the middle of the idealized straight crack is obtained by:

$$ F = l \sigma_{12} $$ \hspace{1cm} (6.9)

where $l$ is the bond crack length. With the point force the mode I and II stress intensity factors of the straight crack are given by (Horii and Nemat-Nasser, 1986):

$$ K_I = \sigma_{11} \sqrt{\pi c} + \frac{F \sin \psi}{\sqrt{\pi (c + c')}} $$

$$ K_{II} = \sigma_{12} \sqrt{\pi c} + \frac{F \cos \psi}{\sqrt{\pi (c + c')}} $$ \hspace{1cm} (6.10)

where $\psi = \beta - \chi$, $\chi$ is the orientation of the straight crack, $c$ is the half length of the representative straight crack, and $c'$ is the convection factor with the value of 0.27l needed to insure that the stress-intensity factors are bounded at the initiation of the wing cracks (Horii and Nemat-Nasser, 1986). The representative cracks are assumed to grow when the mode I stress intensity factor exceeds the macroscopic fracture toughness $K_{IC}$. The length of the straight crack is determined by equating $K_I$ to $K_{IC}$, and the orientation is obtained from maximizing $K_I$ with respect to $\psi$. When a mortar crack nucleates form a bond crack which is subjected to tensile stress normal to its length, the crack will propagate unstably. On the other hand, if the stress field is compressive and the crack slides, the mortar crack grows stably until it becomes unstable at further loading. In this research it is assumed that under tensile loading the unstable propagation of a favorably oriented bond crack directly leads to final failure, whereas under compression the unstable crack is arrested by the neighboring aggregate particles. To predict the compressive failure stress it is necessary to
appropriately model the joining of the microcracks and the formation of continuous cracks. This will not be considered in this research.

6.2.4 Elastic compliance of a damaged concrete

The damaged compliance $S$ can be divided into the original compliance $S_0$ and the additional compliance $H$ generated from the nucleation of the microcracks:

$$S = S_0 + H$$ (6.11)

The plane stress representation of the undamaged compliance is given by the following matrix:

$$[S] = \frac{1}{E} \begin{bmatrix} 1 & -\nu & 0 \\ -\nu & 1 & 0 \\ 0 & 0 & 2(1+\nu) \end{bmatrix}$$ (6.12)

where $E$ and $\nu$ denote the Young's modulus and the Poisson's ratio, respectively. Defining $K$ as the contribution of a single crack to the additional compliance, it can be obtained from:

$$K\sigma = \int \frac{1}{2}(\mathbf{u}\cdot\mathbf{n})(\mathbf{u}\cdot\mathbf{n})d\text{length}$$ (6.13)

where $\mathbf{u}$ is the crack opening displacement with unit normal vector $\mathbf{n}$. When a local coordinate system $x_1'-x_2'$ is attached to the bond crack system such that the origin is located in the middle of the crack and $x_2'$ axis is parallel to the crack length, the crack opening displacements measured along the $x_2'$ axis are:
For open cracks: \[ u_1' = 4\sqrt{l^2 - x_2'} S_{11} \sigma_{11}' \]

\[ u_2' = 4\sqrt{l^2 - x_2'} S_{11} \sigma_{12}' \quad (6.14) \]

For closed crack: \[ u_1' = 0 \]

\[ u_2' = 4\sqrt{l^2 - x_2'} S_{11} [\sigma_{12}' + \mu \sigma_{11}' \text{sgn}(\sigma_{12}')] \quad (6.15) \]

where \( S_{11} \) is the 11 component of the compliance matrix, \( \mu \) is the friction coefficient, and the prime denotes the quantities in the local crack coordinates.

When another local coordinate system \( x_1''-x_2'' \) is attached to the representative straight crack system simplified from the bond crack-mortar crack combination, the crack opening displacements are: (Elvin and Shyam Sunder, 1994):

\[ u_1'' = 4\sqrt{l^2 - x_2''^2} S_{11} \sigma_{11}'' + \frac{4}{\pi} S_{11} \cosh^{-1}\left(\frac{1}{|x_2''|}\right) P \sin \psi \]

\[ u_2'' = 4\sqrt{l^2 - x_2''^2} S_{11} \sigma_{12}'' + \frac{4}{\pi} S_{11} \cosh^{-1}\left(\frac{1}{|x_2''|}\right) P \cos \psi \quad (6.16) \]

The second terms in the right-hand-side of the above equations are contributions from the point force. The expression for \( K \) can be obtained after those equations for the crack opening displacement are substituted to Eq. 6.13. Then the additional compliance is obtained based on the assumption that the initial defects are uniformly distributed from 0 to \( \pi \):
\[ H = \frac{M}{\pi} \int T^T (K'_b + K'_m) T \, d\beta \]  

(6.17)

where \( M = nf_v/\pi d^2 \) represents the number of precursors per unit area assuming that there are \( n \) precursors per aggregate and the volume fraction of the aggregate is \( f_v \). For the determination of the aggregate size, it is assumed that the aggregate is circular in shape with the diameter \( d \). \( K'_b \) is the contribution of an interface bond crack to the additional compliance, and \( K'_m \) is the contribution of a mortar crack. The prime over \( K \) denotes that it is expressed in the local crack coordinates, and \( T \) is the transformation matrix given by:

\[
T = \begin{bmatrix}
\sin^2 \beta & \cos^2 \beta & -\sin 2\beta \\
\cos^2 \beta & \sin^2 \beta & \sin 2\beta \\
\frac{1}{2} \sin 2\beta & -\frac{1}{2} \sin 2\beta & -\cos 2\beta
\end{bmatrix}
\]  

(6.18)

If the size of aggregates are not constant but are uniformly distributed from \( d_{min} \) to \( d_{max} \), then the equation 6.17 becomes:

\[ H = \frac{M}{\pi \delta d} \int \int T^T (K'_{gb} + K'_{mw}) T \, d\beta \, dd \]  

(6.19)

where \( \delta d = d_{max} - d_{min} \)

6.3 Model parameters and numerical results

The material parameters needed in the analysis are: Young's modulus, Poisson's ratio, friction coefficient, and the fracture toughness of the hardened cement paste and the aggregate-paste interface. Some geometric parameters such as volume fraction and size of the aggregate are also needed.
The elastic modulus in compression is generally proportional to the compressive strength. ACI code presents an equation to relate the young's modulus with the compressive strength. Nilson (1987) proposed a modified equation considering the fact that the ACI formula overestimates the modulus for high strength concrete.

Poisson's ratio under uniaxial condition is defined as the ratio of lateral strain to strain in the direction of loading. In concrete it varies ranging from 0.15 to 0.26, with the average value close to 0.2 (Nilson, 1987). In the inelastic range it is an increasing function of axial strain. The Poisson's ratio of high strength concrete in elastic range seems comparable to the values for normal strength concrete. However in the inelastic range, the relative increase in lateral strains is less for higher strength concrete compared with the values for normal strength concrete (Ahmad and Shah, 1987).

The measured value of the fracture toughness of hardened cement paste varies from about 0.2 to 0.5 MPam$^{0.5}$ depending on water-cement ratio, age, etc (Ziegeldorf, 1983). There is a pronounced decrease of $K_{IC}$ with increasing water-cement ratio, which is analogous to the decrease on strength with increasing w/c ratio. In connection with this, it is observed that the fracture toughness is higher in higher strength concrete (Larard et.al, 1987). The matrix strength is reduced when air content of cement paste is increased and the same tendency might be expected for the fracture toughness (Ziegeldorf, 1983). The same reference also confirms that the toughness smoothly increases with loading rate.

The fracture toughness of aggregate is observed to be larger than the corresponding values of hardened cement paste or the interface. The measured values of the interface fracture toughness ranges from about 0.16 to 0.4 MPam$^{0.5}$ (Ziegeldorf, 1983, and Lee, 1993). According to Lee (1993) the fracture toughness of interface for high strength concrete is higher than the corresponding value of normal strength concrete. He also observed that the value becomes higher when aggregate with higher strength is used. It is observed in the numerical prediction of the stress-strain curve that the results matches with
the experimental data when the fracture toughness of the mortar is taken to be one half to
twice the corresponding value of the interface.

In this study the aggregate shape is assumed to be regular hexagon and the size of
the initial defects in the interface is taken to be 50% of the facet length. It is also assumed
that there is one precursor per aggregate. The friction coefficient between the microcrack
faces is taken to be 0.6.

The stress-strain relations obtained from parametric study under uniaxial compression
are shown in Fig. 6.3. Fig. 6.3(a) shows that higher strain is predicted at the same stress
when higher volume fraction of aggregate is used. The results are based on the assumption
that the Young's modulus and the Poisson's ratio are the same in all the cases. The change
in the volume fraction of the aggregate does not affect the stress for microcrack nucleation,
but affects the number of cracks per unit area. Fig. 6.3(b) represents the case for the
change in precursor length. The results show that as the length of the initial defects
becomes smaller the constitutive relation is linear up to higher stress. It can be shown that
once the length of precursors becomes longer than 50% of the aggregate facet length, the
stress-strain curve is not much affected by the change in the precursor length. Fig. 6.3(c)
and 6.3(d) show the effects of the aggregate size and the friction coefficient on the stress-
strain relation. The predicted strain becomes greater as the aggregate size becomes larger
and the friction coefficient becomes smaller. Larger aggregate contains longer precursor,
and the longer precursor makes the nucleation of the bond crack much easier. Similarly
longer bond crack length helps nucleate the wing crack at an smaller stress. It also
increases the magnitude of the point force acting on the representative straight crack. The
easier nucleation of the microcracks makes the stress-strain curve deviate from the linear line
at an earlier stage. The same argument can be applied to Fig. 6.3(d) where the smaller
friction coefficient makes the sliding of the bond crack easier under compressive stress,
causing the prediction of the larger strain.
Fig. 4a to 4c show the stress-strain curves obtained by Tasuji et. al. (1978) and the numerical predictions from the micromechanical model. For all uniaxial and biaxial tests, it was observed in the experiments that failure occurs by tensile splitting, with the fractured surface orthogonal to the direction of the maximum tensile strain. Specifically, under uniaxial compression, fracture occurred by the formation of cracks parallel to the loading direction, and under uniaxial and biaxial tension, failure is by the formation of a single crack perpendicular to the maximum tension direction. In uniaxial compression tests the average Young's modulus and the Poisson's ratio are reported to be about 20 GPa and 0.22, respectively, while in uniaxial tension the corresponding values are about 21 GPa and 0.16. The maximum aggregate size is reported to be 13 mm. For the numerical analysis the fracture toughneses of the interface and the cement paste are taken to be 0.16 and 0.24 MPam^{0.5}, respectively. The volume fraction of the aggregate is taken to be 0.5 for normal strength concrete. Fig. 6.4(a) shows the test data and the numerical prediction under uniaxial compression. Compared with the experimental data, the model prediction is good for up to 70% of the axial strain, and underestimates the experimental data thereafter. Near the failure stress the stress-strain curve deviates rapidly from linearity due to the process of forming continuous cracks, which is not considered in this model. Contrary to the results for the axial strain, the lateral strain predicted from the model overestimates the data from experiment. The computed stress for the first nucleation of the bond crack is 8 MPa, which is about 25% of the failure stress. Thus the model follows the observed phenomenon of the first crack nucleation. Fig. 6.4(b) shows the comparison of the stress-strain curves for uniaxial tension. The same trends also hold in this case: the model prediction underestimates the experimental data for axial strain, overestimates the lateral strain. However, the difference between the model prediction and the experimental data is greatly reduced in this case. The reason for this can be found from the experimental observation that under tensile loading the failure occurs in more brittle manner. Furthermore, the crack density at failure obtained from the model analysis is smaller than
the corresponding value obtained under uniaxial compression. This results conforms with
the experimental observation that the failure is by the formation of a single crack
perpendicular to the major tensile loading. In this analysis the failure stress is obtained
from numerical simulation assuming that the nucleation of the first wing crack directly leads
to failure. Fig. 6.4(c) shows that results under biaxial compression-tension. The lateral
tension is kept to be 25% of the axial compression in magnitude. The model predictions
for both axial and lateral strain start to overestimate the experimental data when the axial
stress reaches about 50% of the failure stress. Fig. 6.5 shows the evolution of compliance
due to damage under the condition used in Fig. 6.4 (a). It can be seen that the lateral and
the shear compliance increase fast compared with the axial compliance. The small increase
in the axial compliance is due to the fact that the most of the open cracks are parallel to the
loading direction.

Fig. 6.6(a) and 6.6(b) show the experimental data of stress-strain curve for high-
strength concrete under uniaxial and biaxial compression, and the predictions using the
model. The reported Young's modulus and the Poisson's ratio are 40 GPa and 0.2,
respectively. The aggregate sizes are distributed from about 5 to 19 mm in diameter, and
the volume fraction of the aggregate is reported to be 0.39. For numerical analysis, the
fracture toughnesses of the interface and the cement paste are taken to be 0.3 and 0.45
MPam$^{0.5}$, respectively. Compared with the results for the normal stress concrete the
observed stress-strain curve is closer to the linear line, and the model predictions of the
stress-strain curve under compression is much better in this case. This is due to the fact
that as the strength of concrete goes up the nucleation of interface bond cracks is delayed
(up to 50% of the failure stress), and is reduced in quantity. As a result the failure mode
becomes more brittle and matches with the model assumption.

6.4 Concluding remarks
In this study a micromechanical model is used to predict the stress-strain relation of concrete. The model prescribes a initial defect in a aggregate-segment paste interface, which will subsequently nucleate into a interface bond-crack. The bond crack will grow into the cement paste stably (under compression) or unstably (under tension) upon further loading. The bond crack-mortar crack configuration is idealized by the straight crack with a point force. The nucleation and growth of cracks are based on the maximum principal stress criterion, and the nonlinear stress-strain curve can be obtained from the damage due to crack opening of both the interface bond crack and the mortar crack. According to the parametric study, the strain increases as the aggregate size and volume fraction increase. The predicted stress-strain curves are compared with experimental data and the numerical predictions are in good agreement with the experimental data. The model predictions are better for high-strength concrete which shows more linear stress-strain relation and brittle failure mode. Under tensile loading condition the stress for the unstable propagation of a wing crack (mortar crack) may be taken as the failure stress, whereas under compression this argument does not hold for the following reason. According to the experimental observation (Zeitsev, 1983) the failure of concrete under uniaxial or biaxial compression is not caused by the unstable propagation of single crack but by the linkage of many cracks to form continuous cracks in a more stable manner. In this research this phenomenon is not taken into account and thus the compressive failure stress can not be predicted.
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Fig. 6.1 Schematic of microcracks: (a) location of a initial defect; (b) formation of a bond crack along the boundary; (c) growth of a mortar crack; (d) idealization of the crack system to a straight crack with a point force.
Fig. 6.2 Global and local coordinate system
Fig. 6.3 Parametric study of stress-strain curve with: (a) volume fraction of aggregate; (b) precursor length
Fig. 6.3 Parametric study of stress-strain curve with: (c) aggregate size; (d) friction coefficient
Fig. 6.4 Stress-strain curve of normal strength concrete under: (a) uniaxial compression; (b) uniaxial compression
Fig. 6.4 (c) Stress-strain curve of normal strength concrete under biaxial compression-tension
Fig. 6.5 Evolution of compliance under uniaxial compression (E=20GPa, Poisson's ratio=0.22)
Fig. 6.6 Stress-strain curve of high-strength concrete under: (a) uniaxial compression; (b) biaxial compression
CHAPTER VII

RECOMMENDATION FOR FURTHER RESEARCH

7.1 Modeling of failure mode and creep-crack interaction

Some of the interesting topics associated with the failure of quasi-brittle material are: (i) the process of coalescence of microcracks and failure mode; (ii) the interaction between a macrocrack and the damaged material surrounding it; and (iii) the interaction between creep and fracture mechanism.

The coalescence of two cracks is dependent on the following factors: the stress field around them, their distance of separation, and local material characteristics such as crystallofrapjic orientation and grain boundaries. This problem may be modeled by a distance criterion of coalescence in the numerical simulations. Such a criterion would permit coalescence if the physical separation between two crack tips becomes less than a characteristic microstructural dimension and the stress intensity factors exceed the critical value at both crack tips. The coalesced cracks can be analyzed as touching cracks, or replaced by an equivalent crack to ensure simple geometry for subsequent analysis. The process can be visualized if the graph model is used, and this may lead to predict the localization pattern and the failure mode.

The interaction between a macrocrack and the material surrounding it that has been pre-damaged by distributed microcracking is a common occurrence in the field and an analysis of the problem will provide guidance on the extent of toughening to be expected from the pre-damaged material surrounding the crack-tip. The phenomenon of microcrack toughening has been extensively investigated for ceramics and cementitious materials (Evans, 1984; Shah, 1991) but remains to be studied in the case of ice.
The creep deformation around the crack-tip is known to strongly affect the experimentally measured fracture resistance of some materials such as polycrystalline ice. The mechanisms responsible for this interaction are at present unknown. Traditional fracture toughness tests on ice use the results of Reidel and Rice (1980) to predict the creep zone size and to ensure that this zone is small enough in order for linear elastic fracture mechanics to be valid. Unfortunately, the Ridel and Rice (1980) analysis is for a material following an isotropic, steady state power law theory of creep which is inappropriate for ice. The inelastic deformation in the crack-tip zone for ice is dominated by transient rather than steady state creep and in non-isotropic ice the effects of creep anisotropy on the size of the creep zone can be significant. The physically-based constitutive theory may be used to study the role of internal state variable models of transient creep, including creep anisotropy, on the behavior of stationary and growing cracks in ice.

7.2 Modeling of ice-structure interaction

The integrated pressure on a structure as well as the distribution of contact stresses along the ice-structure interface are required for both indentation and penetration problems. Experimental data on these pressures display a strong scale effects, and the results of uniaxial strength tests conducted in the laboratory and empirical data from small-scale indentation tests (Sodhi, 1989) indicate that the maximum ice pressures are encountered in the ductile-to-brittle transition regime of loading rate involving both creep flow and fracture. The transition in general is associated with the simultaneous occurrence of multiple failure modes. Some of the failure modes are critical in determining local ice pressures; while others are important in determining global pressures. For example, compressive crushing may dominate the mode of local failure in the vicinity of the interfacial contact between ice and structure while bending or large scale cracking may dominate the global failure mode of the ice floe.
The strain rate gradient induced in the ice due to the presence of a structure, in turn, will lead to a space-time variation in the constitutive properties including the effect of confinement in ice. Close to the structure where the strain rates are greatest and in the transition range, structure may be dominated by transient creep, while far away from the structure the ice is relatively undeformed and displays elastic behavior. The effect of confinement will be greatest in the crushing zone because at the higher rates of loading typical of the transition regime the strength of ice is highly pressure sensitive. For large values of aspect ratio, a plane stress condition exists in the ice and confinement effects are small. For small values of aspect ratio, in contrast, a plane strain condition exists and the ice is subject to significant confinement. This variation in confinement can be a significant factor in ice pressure scaling with aspect ratio as has also been recognized recently by Dorris (1989).

The degree of confinement also varies spatially in the ice flow, especially along the ice-structure interface. Consequently, crushing will initiate pointwise along the contact at which the strain rates are greatest and confinement is smallest. The crushing front will extend in time to envelope the entire interface zone; the crushed material is extruded as deformation proceeds. The process then repeats itself, and this repetitive crushing and extrusion can give rise to large fluctuations in ice pressure with time.

Previous study (Sodhi, 1989) shows that the crushing mode of failure represent an upper bound on ice pressures at indentation rates typical of the ductile-to-brittle transition regime and for a wide range of aspect ratios and contact areas. This is particularly true for local contact pressures. A lower bound on the ice pressures allowing for potential macrofractures due to bending failures and large scale cracking may be studied with the discrete element method of analysis.

7.3 Modeling of crack growth in concrete
Once a mortar crack forms, it keeps growing upon further loading, until it confronts with a neighboring aggregate. It is observed from experiments that mortar cracks go around aggregates when the fracture toughness of the aggregates is greater than that of the interface, and may go through the aggregate when the condition is reversed. In Ch. 6 the constitutive relation of concrete is obtained assuming that the isotropically distributed cracks are imbedded in an infinite medium. Some of the assumptions can be removed if the graph model used in Ch. 4 is used, where the initial defects are placed in a finite medium and the interaction effects can be taken into account.

The micromechanical graph models presented in Ch. 4 represents the stress-strain field in concrete with averaged values, and cannot truely account for the inhomogenous nature of the aggregate-cement paste composite.

A more precise modeling of the composite medium can be realized by using the finite element method, although complicated mesh generation is needed and many elements are required to simulate the random distribution of aggregates in the cement paste matrix. The aggregates and matrix can be assigned with elements having corresponding Young's moduli. When a matrix crack approaches an aggregate, whether it penetrates or goes around the aggregate can be determined by considering the fracture toughnesses of each material, the angle of the crack to the surface of the aggregate, etc. The failure of a concrete specimen can be determined after some mortar cracks are connected to form a continuous crack through the specimen. This type of problem needs further investigations.

7.4 Recommendation for experimental data

Some experimental data are needed to verify the numerical results:

1. Evolution of compliance.
2. Statistical variation of the compliance.


5. Number of grain boundary dislocations piled up in a triple point.

6. The size of initial defects.

7. The number of initial defects found in single aggregate.
References


