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Phase Field Fracture Modeling of Chemically Strengthened Glass

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PHASE FIELD FRACTURE MODELING OF CHEMICALLY STRENGTHENED
GLASS

By
Parag Nikam

A REPORT

Submitted in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

In Mechanical Engineering

MICHIGAN TECHNOLOGICAL UNIVERSITY

2020

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This report has been approved in partial fulfillment of the requirements for the Degree of MASTER OF SCIENCE in Mechanical Engineering.

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List of Abbreviations

UEL	User Element Subroutine
UMAT	User Material Subroutine
XFEM	Extended Finite Element Methods
CS	Compressive Stress
CT	Central Tension
SDV	Solution Dependent Variable
DOF	Degrees of Freedom
Lc	Length Scale Parameter
Dol	Depth of Layer

Abstract

The objective of the report is to implement the phase field model in Abaqus standard to compute the fracture properties of a glass strengthened by an ion-exchange process. Implemented the phase field model which is based on the rate-independent variational principle of diffuse fracture in Abaqus standard software using the UEL and UMAT subroutines. SDVINI subroutine is used to give the residual stress or prestress conditions to simulate the stress profile of strengthened glass. Studied the effect of parameters such as length scale parameter and step size and the optimum parameters are selected. The experimental model of chemically strengthened glass is explained with analytical calculations to compute the stress intensity factor. Compared the effect of depth of the residual stress layer on the stress intensity factor. Stress intensity factor is calculated using the finite element analysis model and results are compared with the experimental and analytical model.

Chapter 1

Introduction

Prediction of crack initiation and propagation path is an important part in fracture mechanics that is used by engineers and scientists to avoid the failure of engineering materials and improve the mechanical components. The initial theory of fracture mechanics for brittle materials was introduced by Griffith[1]. Later, Irwin[6] introduced the stress intensity factor to accommodate the plasticity in the fracture mechanics. Fracture mechanics is an active field of research with many numerical models and theories that have been developed in recent years to simulate the crack initiation and growth.

1.1 Phase Field Model

Finite element models used for fracture mechanics are broadly classified into two categories as discrete crack model vs diffused crack model. The early discrete crack model involves the modification of mesh according to the evolution of crack topology. This model was derived from the work of Ngo and Scordelis[5]. This early implementation of crack geometry in finite element has a high dependency on the mesh as crack geometry is accomplished by node splitting. The problem of mesh dependency was addressed by Ingraffia[13] by introducing automatic re-meshing according to the crack evolution. Another method used to avoid mesh dependency involved varying cohesive elements strength[10]. Due to constraining crack propagation along element edges, the crack path deviates from an actual crack path which results in the over estimation of fracture energy.

The extended finite element method(XFEM) was developed by Belytschko[12] which uses the method of enrichment in a partition by unity. In the XFEM method, enrichment function is added in existing shape function, also crack is implicitly modeled which results in a crack to propagate independently of underlying mesh. This method has many advantages such as resolving the stress singularities at the crack tip and obtaining actual stress behavior. But, the drawback of the XFEM method is that

for a single crack requires a pair of level set functions for the definition of its topology, so that computational complexity increases with the number of individual crack segments, also the problem size increases due to the additional degrees of freedom.

On the other hand, a diffused crack method is used to overcome the shortcomings of a discrete crack method. The phase-field is one of the diffused crack model in which a crack evolution can be simulated using standard finite element method without modification of the initial mesh. The initial diffuse crack model was introduced for a concrete application. In recent years, phase-field methods for fracture have been gaining popularity. Phase-field methods is based on a variational theory of fracture. This is a relatively recent concept, being developed to overcome limitations associated with the classical Griffith theory such as its inability to predict crack initiation and branching, and simulate curved crack paths. In the variational theory, the total energy potential includes elastic potential energy with the energy required for the formation of a crack. This energy potential is then simultaneously minimized for both the parts. Here, the fracture topology evolution occurred in such a way that results in minimal potential energy.

Significant contributions to the theory were also made by Miehe[3] in the form of a thermodynamically consistent model for brittle mode-I fracture. A staggered scheme is used in which an energy history field is introduced to ensure irreversible crack growth. This method is implemented in the Abaqus standard using the user element

and user material subroutine.[8][11] In this work we applied the phase-field model to a glass strengthened by the ion-exchange process. We implemented the phase-field model in Abaqus standard using the staggered scheme using uel. In addition, we incorporated the residual stress profile generated during the chemical strengthening of a glass using a subroutine. The chemical strengthening of glass is briefly explained in the next section.

1.2 Strengthened Glass

Glass has a wide range of applications and many applications require glass with high strength. Glass can be strengthened using different methods such as lamination, providing interlocking micro-architecture, thermal strengthening, and chemical strengthening. For a thin sheet of glass chemical strengthening gives desired strengthening properties at a desirable location.

For chemically strengthening, glass is submerged in a molten bath of potassium nitrate salt.[2] Temperature kept high enough to pass the activation energy of the glass. During this process sodium ions are escaped from glass and replaced by potassium ions. The size of potassium ions is larger than the sodium ion. This process of replacing small ions with larger ions results in compressive stress generation in the glass. The amount of compressive stress generated affect the toughness of the glass.

This compressive residual stress is generated at the boundary of the model where the possibility of an existing crack is high. The amount of residual stress and depth of stress layer can be controlled by the ion-exchange process. Due to residual stress, the crack has to overcome the residual stress in addition to fracture stress to propagate further which results in the strengthening of the glass.

In the present work, we implemented the phase-field model for simulating brittle fracture of strengthened glass within the Abaqus software using UEL and SDVINI subroutines. The report is organized as follows: In Section 2, the phase-field method is explained in detail with the minimization equations and staggered scheme for solving the minimization problem. The experimental model and analytical model is explained in section 3. Section 4 explains the Finite element model. Sensitivity analysis is performed and the model is then applied to measure the fracture properties of glass and the results are compared with the experimental and analytical results in Section 5. Section 6 includes concluding remarks.

Chapter 2

Phase Field Model

2.1 Phase Field

Considering a 1d bar element with crack at the middle. Fig 2.1 a shows the sharp crack with the value of $d(x)$ being zero everywhere and 1 at crack location. Therefore, it is fully broken when value of $d(x)$ reaches 1. To represent diffused crack topology an exponential function is used as

$$d(x) = e^{-|x|/l_c} \quad (2.1)$$

where, l_c is the length scale parameter. Here d represent the diffused crack topology

with value of d reaches 1 for fully broken part. As length scale parameter goes to zero sharp crack topology can be recovered. Limits for the function are $d(0) = 1$ and at the limits $d(\pm\infty) = 0$.

$$d(x) - l_c^2 d''(x) = 0 \quad (2.2)$$

The variational principle strong form can be written as,

$$d = \text{Arg} \left\{ \inf_{x \in W} I(d) \right\} \quad (2.3)$$

where,

$$I(d) = \frac{1}{2} \int_{\Omega} (d^2 + l_c^2 d'^2) dV \quad (2.4)$$

the integration over volume $dV = \Gamma dx$ gives $I(d = e^{-\frac{|x|}{l_c}}) = l_c \Gamma$. Thus, we can introduce a fracture surface density with the help of the phase-field function by:

$$\Gamma(d) = \frac{1}{2l_c} \int_{\Omega} (d^2 + l_c^2 d'^2) dV = \int_{\Omega} \gamma(d, d') dV \quad (2.5)$$

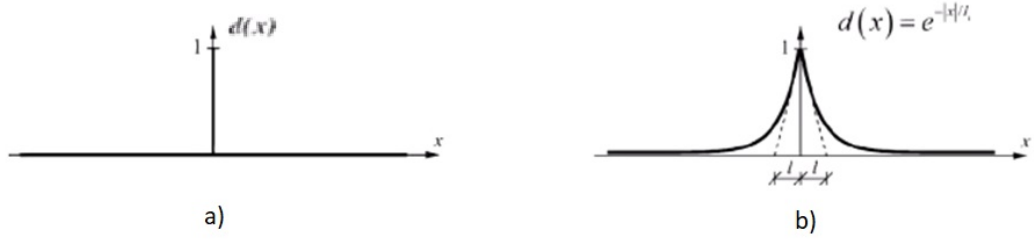


Figure 2.1: 1d bar a)sharp crack b)diffused crack

$\gamma(d, d')$ is fracture surface energy density, for multiple dimensions it can be written as

$$\gamma(d, \nabla d) = \frac{1}{2l_c} d^2 + \frac{l_c}{2} |\nabla d|^2 \quad (2.6)$$

The total potential energy of a body with a crack is computed as combination of elastic and fracture surface energy

$$\Pi^{int} = E(u, d) + W(d) \quad (2.7)$$

First part of total potential energy is elastic strain energy

$$E(u, d) = \int_{\Omega} \psi(\epsilon(u), d) dV \quad (2.8)$$

where, $\psi(\epsilon(u), d)$ is the potential energy density which is computed as

$$\psi(\epsilon, d) = g(d) \cdot \psi_0(\epsilon) \quad (2.9)$$

$\psi_0(\epsilon)$ is the elastic strain energy while $g(d)$ is a degradation function of phase field.

$$g(d) = (1 - d)^2 + k \quad (2.10)$$

Where, k is the stability parameter with very small value

Second term in total potential energy is due to fracture which is calculated by multiplying energy release rate (g_c) to all fracture surfaces.

$$W(d) = \int_{\Omega} g_c \gamma(d, \nabla d) dV \quad (2.11)$$

External component of energy can be computed as follows:

$$\Pi^{ext} = \int_{\Omega} \bar{\gamma} \cdot u dV + \int_{d\Omega} \bar{t} \cdot u dA \quad (2.12)$$

Where, γ and t are volume and boundary forces respectively.

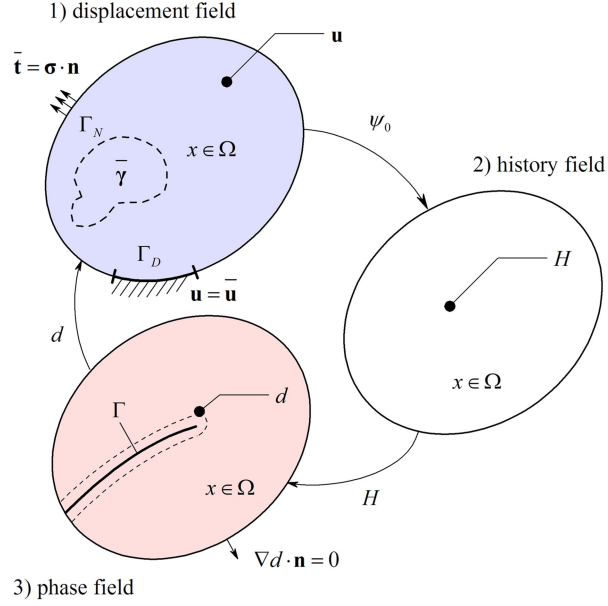


Figure 2.2: The split scheme in phase field model[11]

2.2 Staggered Scheme

The minimization problem is split into two quasi independent minimization problems to have a stable implicit model. Figure 2.2 illustrate the split scheme used in the phase field model.

The fracture topology part is formulated as the following functional:

$$\Pi^{int} = \Pi^d = \int_{\Omega} [g_c \gamma(d, \nabla d) + (1 - d)^2 H] dV \quad (2.13)$$

Where, H is history field.

Value of H_n is taken from the energy history calculated at the nth step. The history field is a important parameter to couple the two minimization problems.

$$H = \begin{cases} \psi_0(\epsilon) & \text{if } \psi_0(\epsilon) > H_n \\ H_n & \text{otherwise} \end{cases} \quad (2.14)$$

Displacement field is calculated as follows:

$$E(u, d) - \Pi^{ext} = \Pi^d = \int_{\Omega} [\psi(u, d) - \bar{\gamma}.udV - \int_{d\Omega} \bar{t}.udA \quad (2.15)$$

equ(2.10) and eq (2.13) are solved independtly. Strong form for the equations can be computed by taking variation of both equations.

$$\Pi^d = 0, \Pi^u = 0$$

The two minimization problems are solved separately using the Newton Raphson Method in Abaqus. The history and the phase-field is updated in the first iteration at every load step. The phase field equation is solved based on the History Field calculated from the energy history of previous step while displacement is calculated from phase value of previous step. This staggered scheme is explained in previous work of Molnar et al[]

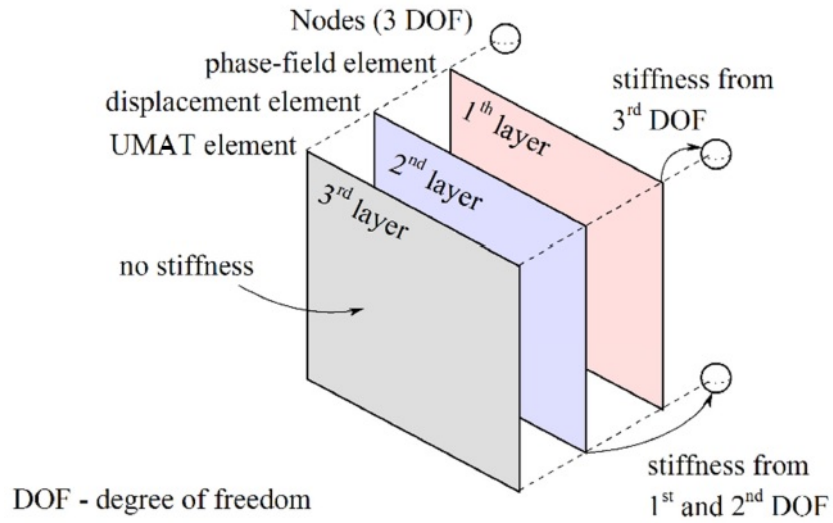


Figure 2.3: Three layers in Abaqus model[11]

The equations are implemented in Abaqus using the two layers of elements with different degrees of freedoms while the third layer is used to visualize the results. Figure 2.2 shows the layered structure used in abaqus. All elements are connected at the same nodes. First layer of elements has one phase field DOF. Second layer of elements has the two transnational DOF. To visualize the calculated SDVs from UEL the third layer of UMAT elements with infinitesimally small stiffness is used.

Chapter 3

Experimental And Analytical Model

3.1 Experimental Model

Experimental model was created with glass of known composition and materials properties by chemically (ion-exchange) strengthening to obtain different levels of residual stress profile.

In chemically strengthening process glass is submerged in a molten bath of potassium nitrate salt at a certain temperature high enough to overcome the activation energy of glass. During this process sodium ions are escaped from glass and replaced by the

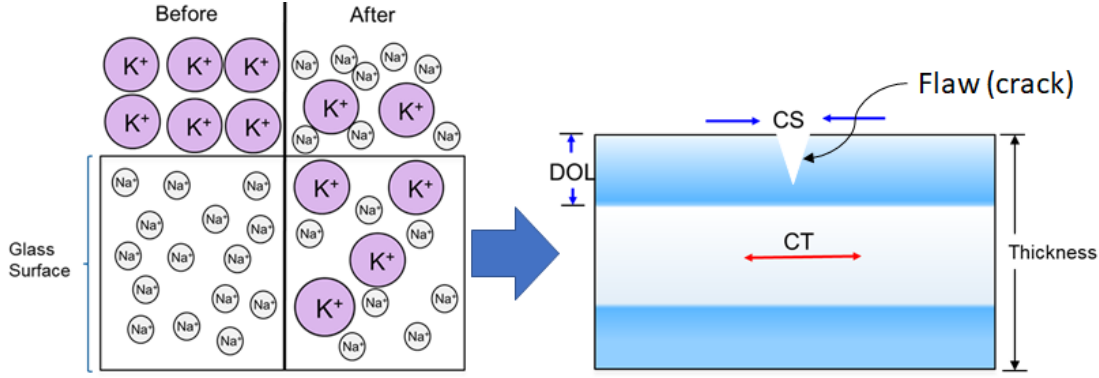


Figure 3.1: Representation of ion-exchange process and formation of residual stress profile in glass

potassium ions as represented in figure 3.1. Due to the large size of potassium ions compared to sodium ions compressive stress is generated in the glass. this compressive residual stress results in the toughening of the glass. This compressive residual stress is generated at the top and bottom part of the glass where the possibility of an existing crack is high. The amount of residual stress and depth of stress layer can be controlled by the ion-exchange process. The compressive residual stress distribution and central tension zone formed due to the ion-exchange procedure is shown in figure 3.2. Due to the residual stress, for crack to propagate it has to overcome the inherent strength of the glass as well as the residual stress. The stress intensity factor is used to measure the strength of the glass. The total stress intensity factor of a strengthened glass is computed as a summation of fracture toughness of glass and stress intensity factor due to the residual stress. Equation 3.1 shows that crack will propagate if the stress intensity factor of strengthened glass is more than the apparent fracture toughness.

$$K_{Ic}^a \geq K_{Ic} + K_R \quad (3.1)$$

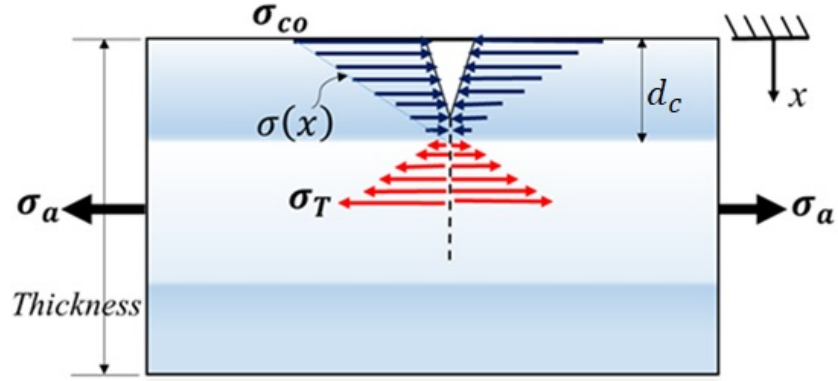


Figure 3.2: Linear residual stress profile generated in the model

Ring on ring test was performed to calculate the strength and stress intensity factor (K_{IC}). The stress intensity factor was obtained to compare the effect of different parameters such as flaw size, compressive residual stress and depth of layer on the strength of the glass.

3.2 Analytical Calculations

3.2.1 Green Theorem Approach

Figure 3.2 shows the stress distribution in the model. According to Marcelli et al. 2018, intensity factor is considered as a combination of (normal) stress intensity factor and residual stress intensity factor. This model assumes the conservation of crack during the ion-exchange process. Considering linearly varying stress profile:

$$\sigma(x) = -\sigma_{co} \left(1 - \frac{x}{d_c}\right) \text{ if } x \leq d_c \quad (3.2)$$

$$\sigma(x) = \sigma_T \text{ if } x \geq d_c \quad (3.3)$$

$$K_r = \frac{Y\sqrt{c}}{\pi c} \int_0^c \sigma(x)g(x)dx \quad (3.4)$$

Where, $g(x)$ is a green's function

$$g(x) = \frac{2c}{\sqrt{(c^2 - x^2)}} \quad (3.5)$$

3.2.2 Crack Tip Residual Stress Approach

In the crack tip residual stress approach, residual stress at the tip of crack is measured which is used in the following equation to calculate the apparent stress intensity factor. In this approach, only residual stress at tip is considered for resisting crack propagation. Therefore, this equation gives same value of stress intensity factor for crack size larger than depth of layer.

$$K_{Ic}^a = K_{Ic} + \sigma_{rc}Y\sqrt{c} \quad (3.6)$$

Where σ_{rc} is the residual compressive stress at the crack tip

Chapter 4

Finite Element Model

Finite element model is created in Abaqus. Strength of glass can be measured by different methods such as 3 point bend test, ring on ring test, 4 point bend test, drop test. 2D 3 point bend test is performed here and solved in Abaqus standard solver to measure the strength. Model geometry of 50mm X 0.8mm is created which is taken from the experimental setup.

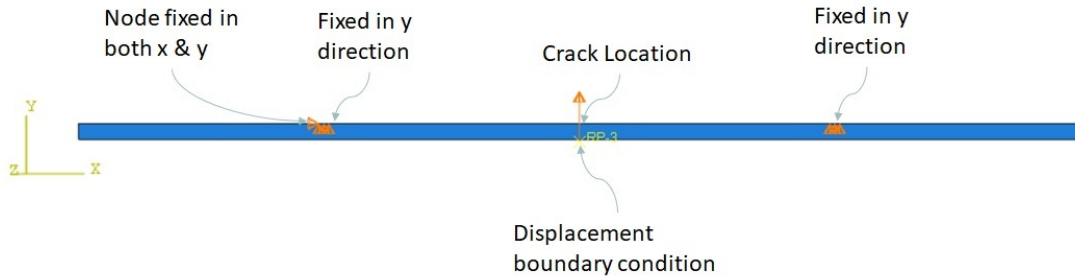


Figure 4.1: Boundary conditions in Abaqus

4.1 Pre-Processing

4.1.1 Boundary Conditions

A standard 3 point bend test is performed to measure the fracture strength of the glass. Figure 4.1 shows the model and boundary conditions. Side edge crack is located at the center of the model while displacement boundary condition is applied at the center on the opposite side of the crack in y-direction. Displacement is given at a constant rate. Both support positions are fixed in y-direction with left support point fixed in x-direction for stability of the model. The support span is taken from experimental setup as 25mm.

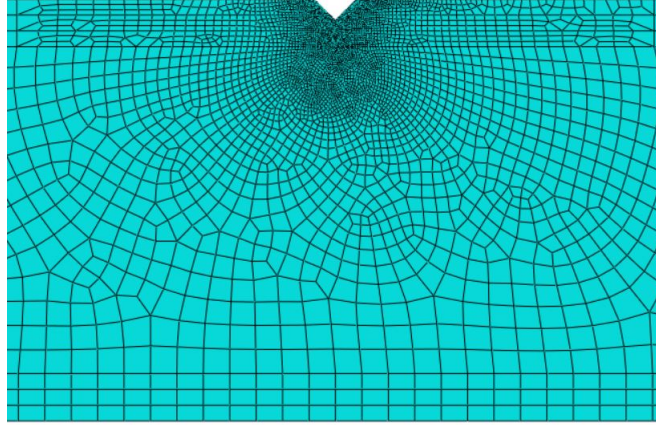


Figure 4.2: Meshing (refined mesh near crack)

4.1.2 Meshing

A 4-node bi-linear plane stress element is used. The region around the crack tip is refined. Total of 14,000 elements are used with a smallest element size of 0.001mm. The smallest element size is used near the crack tip. This element size is considered for selection of length scale parameter. 4.2 shows the meshing on the model and mesh refinement near the crack.

Chapter 5

Results

5.1 Sensitivity Analysis

Decoupled solution significantly affect the time dependent response therefore, performing sensitivity analysis is important. Here, Sensitivity analysis is performed for a length scale parameter and a load increment rate. The sensitivity test is performed on the model without initial residual stress. Edge crack specimen is used to study the effect of load step and length scale parameter. The following model material properties are used

Keeping the step size constant value of l_c is changed to measure the effect of length scale parameter. As length scale parameter decreases sharp crack topology can be

Properties	Value
Young Modulus E	68 kN/mm^2
Poisson's Ratio ν	0.23
Fracture Energy g_c	$6.4 \times 10^{-3} \text{ N/mm}$
Stability Parameter k	1×10^{-7}

Table 5.1
Material Properties

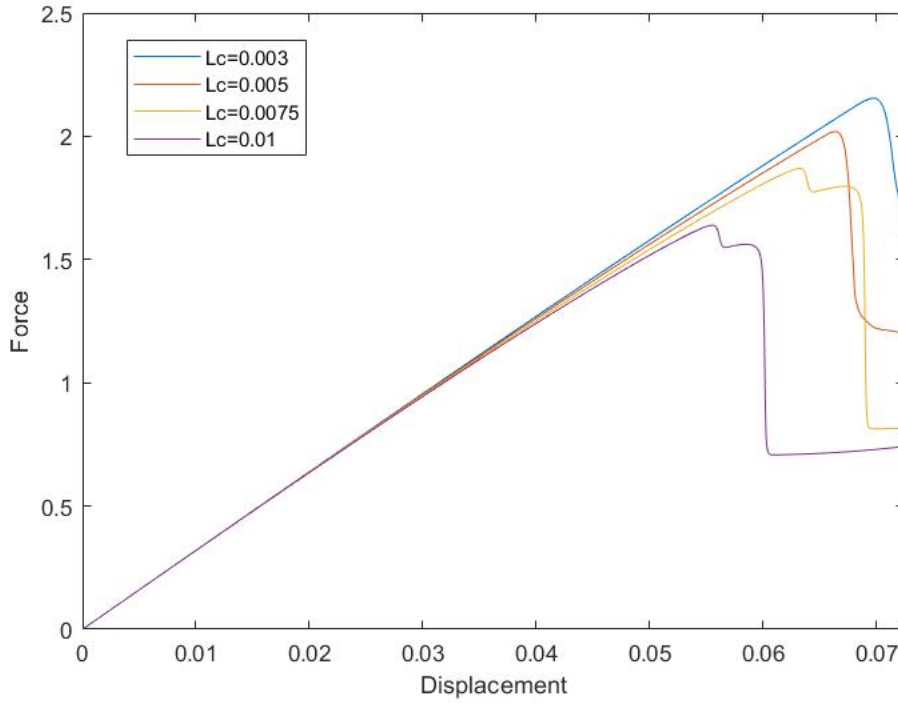


Figure 5.1: Sensitivity analysis of length scale parameter

obtained. Figure 5.1 shows maximum reaction force increases as decrease in the length scale parameter. For $l_c = 0.0075$ the maximum reaction force is 1.8 N which is in the agreement with the experimental results.

Similarly, sensitivity analysis of time step size is performed by keeping the length scale parameter constant. For large step size Newton-Raphson solver fails to find

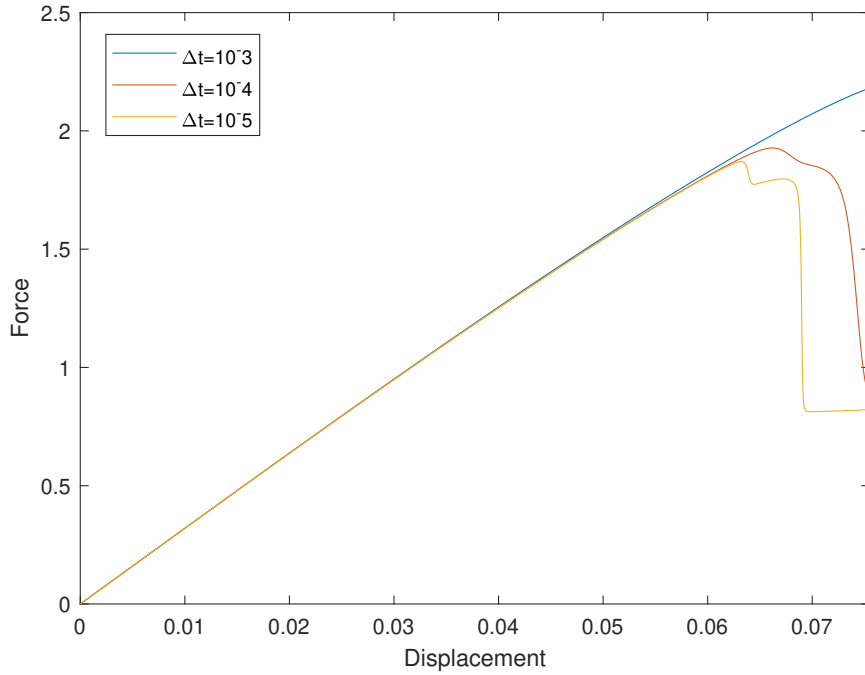


Figure 5.2: Sensitivity analysis of step size

the local equilibrium which results in the higher values of maximum reaction force. Figure 5.2 shows if step size is increased maximum reaction force increases. For step size of $\Delta t = 10^{-4}$ maximum reaction force obtained as 1.8 N which match with the experimental model. This sensitivity analysis is performed to determine the values of length scale parameter and step size for the further analysis.

5.2 Effect of residual stress

Residual stress is incorporated in the model using the predefined field in Abaqus standard. SDVINI subroutine is used to provide the linearly varying residual stress

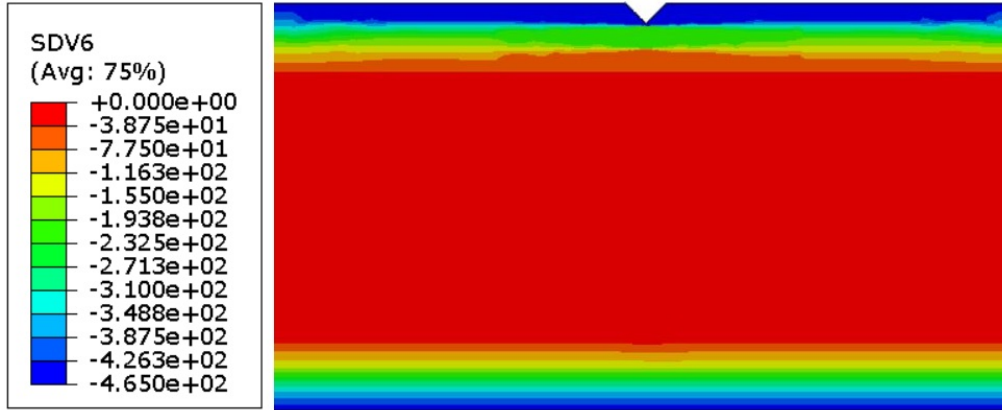


Figure 5.3: Residual stress profile for $DOL = 134\mu m$ and $CS = 465$ MPA

field. Figure 5.3 shows the residual stress profile defined in the initial step of the simulation with depth of layer of $134\ \mu m$ and compressive stress of 465 MPa on the boundary of the model. Figure 5.4 compares the stress profile of glass in three point bend test with residual stress. Crack propagation is delayed in the strengthened glass. For crack to propagate in strengthened glass, it has to overcome the residual stress in addition to the inherent fracture stress. Further stress intensity factor is calculated to measure the fracture strength of the glass. Also, the stress intensity factor obtained by the FEA model is compared with the experimental and analytical models.

5.3 Stress intensity factor

Three point bend test is used to measure the strength of the glass. Displacement boundary condition is given at the center at the opposite side of the crack. Reaction force is measured at the loading point and reaction force at fracture is taken for the

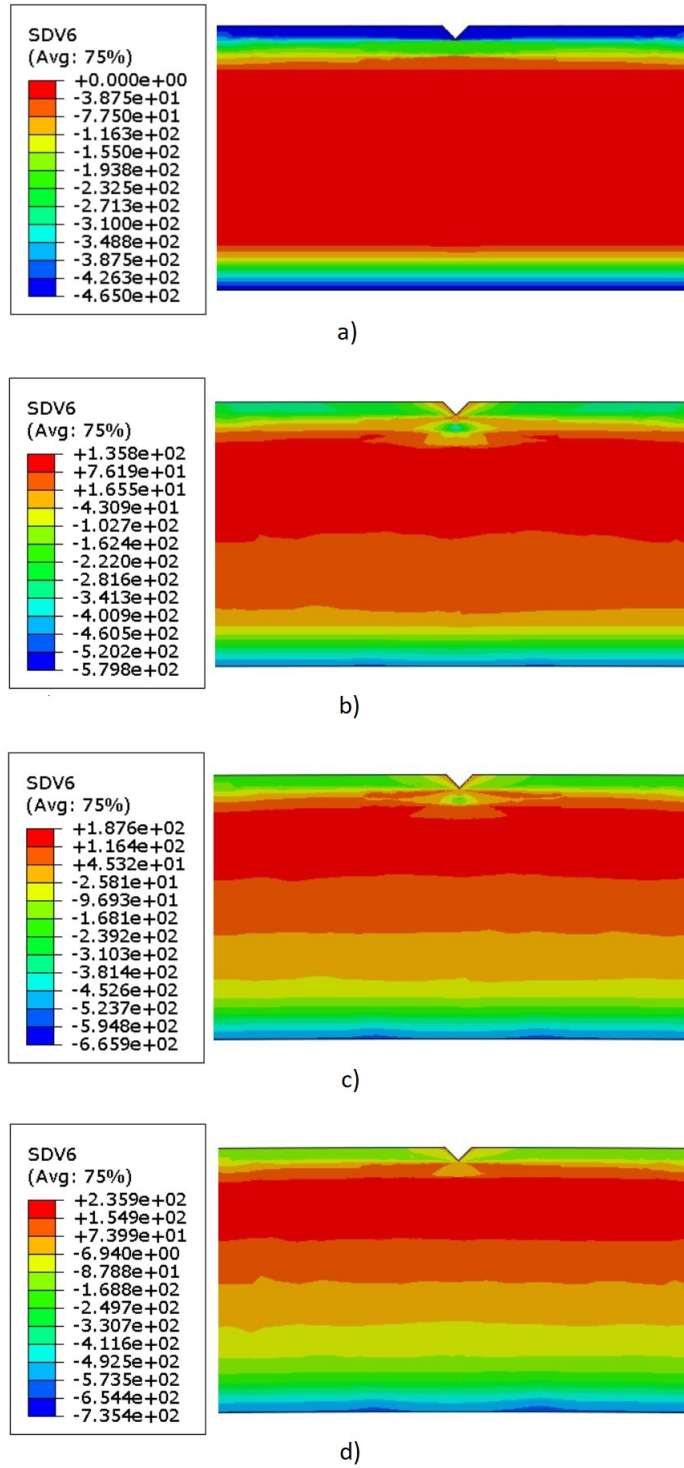


Figure 5.4: Stress evolution with $d_{ol}=134\mu m$ and $c_s=465Mpa$ a) $disp=0$, residual stress b) $disp=0.1$ c) $disp=0.2$ d) $disp=0.3$

calculation of a flexural stress. Flexural stress generated due to three point bend test is calculated as:

$$\sigma_a = \frac{3FL}{2bd^2} \quad (5.1)$$

Where,

σ_a = Flexural stress, (MPa)

F = Fracture load, (N)

L = Support span, (mm)

b = Width, (mm)

d = Thickness, (mm)

This flexural stress is used to calculate the stress intensity factor for the model.

$$\sigma_a = \frac{K_{Ic}}{Y\sqrt{c}} \quad (5.2)$$

Where,

Y = Shape factor

c = Crack length (m)

Figure 5.4 shows the effect of depth of residual compressive stress on the stress intensity factor. Here, compressive stress is kept constant and d_{ol} is increased. As the d_{ol} increased the value of stress intensity factor also increases. Crack opening is resisted due to the compressive residual stress near the crack tip. This results in the

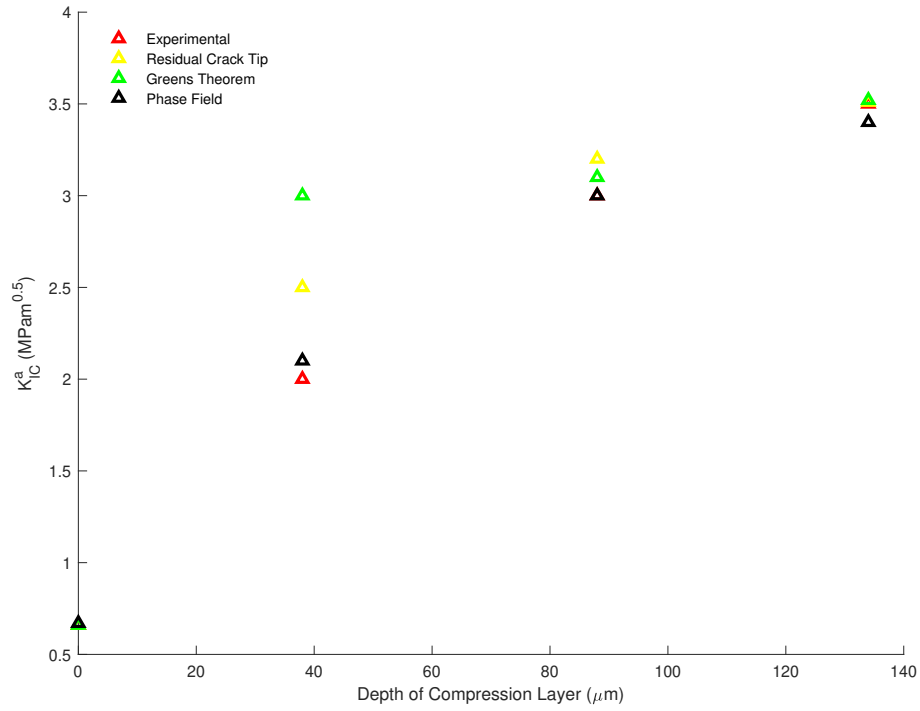


Figure 5.5: Stress intensity factor vs depth of compression layer

toughening of the glass. The values match with the experimental values. With this model we can predict the fracture toughness for different values of residual stress. Similarly, Effect of amount of residual stress on the stress intensity factor can be measured by keeping the d_{ol} constant. This finite element model is useful for selecting optimum values of compressive stress and depth of layer to obtained the required material strength.

Chapter 6

Conclusion

In this study, the phase field model with residual stress is implemented in Abaqus to measure the fracture properties of a strengthened glass. Phase field model is computationally easy and stable model for predicting fracture properties and crack propagation. Length scale parameter is one of the important parameter in the phase field model. Value of length scale parameter for the model is reversely identified using the experimental results. Finite element analysis results match closely with the experimental and analytical results. We implemented the residual stress using the SDVINI subroutine. Linearly varying residual stress profile is achieved using the subroutine.

Stress intensity factor has been computed using the phase field model and compared

the values for different parameters of chemically strengthened glass such as amount of initial compressive stress, depth of compression zone and initial crack geometry. Increase in compressive residual stress near crack tip results in the increase of stress intensity factor. Similarly, stress intensity factor increases with the larger depth of layer. The right combination of Compressive stress, depth of layer and central tension can be selected using this finite element model to obtain the optimum strength. Additionally, this Finite element model can be used to study the effect of different crack geometries and crack propagation. Further, a 3D phase field model can be created to simulate the physical model to study the crack propagation path in all directions.

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Appendix A

Input file code for pre-stress

**

**Predefined FIELD

**

*Initial Conditions, type=SOLUTION, USER

**

Appendix B

Solution dependent variables

Solution dependent variables are summarized in the following table:

Displacement (stress-strain) element	
Displacement – u_x, u_y	SDV1-SDV2
Axial strains – ϵ_x, ϵ_y	SDV3-SDV4
Engineering shear strain – γ_{xy}	SDV5
Axial stress – σ_x, σ_y	SDV6-SDV7
Shear stress – τ_{xy}	SDV8
Elastic axial stress – $\sigma_{x,0}, \sigma_{y,0}$	SDV9-SDV10
Elastic shear stress – $\tau_{xy,0}$	SDV11
Strain energy – ψ	SDV12
Elastic strain energy – ψ_0	SDV13
Phase-field – d	SDV14
Phase-field element	
Phase-field – d	SDV15
History field – H	SDV16

Figure B.1: SDVs used in phase field model and corresponding properties