PHASE FIELD MODELING OF SHEAR YIELDING AND CRAZING IN GLASSY POLYMER

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By Yunzhe Mao

Entitled

PHASE FIELD MODELING OF SHEAR YIELDING AND CRAZING IN GLASSY POLYMER

For the degree of Master of Science in Mechanical Engineering

Is approved by the final examining committee:

Marisol Koslowski

R. Byron Pipes

Alejandro Strachan

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Approved by Major Professor(s): Marisol Koslowski

Approved by: David Anderson 01/15/2014

Head of the Graduate Program Date
PHASE FIELD MODELING OF SHEAR YIELDING AND CRAZING
IN GLASSY POLYMER

A Thesis
Submitted to the Faculty
of
Purdue University
by
Yunzhe Mao

In Partial Fulfillment of the
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of
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ABSTRACT

Yunzhe Mao. M.S.M.E., Purdue University, May 2014. Phase Field Modeling of Shear Yielding and Crazing in Glassy Polymer. Major Professor: Marisol Koslowski, School of Mechanical Engineering.

Glassy polymers are very important in industrial and commercial components manufacturing. For instance, it is used to manufacture polymer-matrix composites, the type of composite used in the Dreamliner 787. But this kind of material is also limited by its tendency to fail in brittle manner. In this study, we use phase field model to characterize the yielding condition of glassy amorphous polymer under a wide range of loading conditions. The main failure mechanisms in amorphous glassy polymers, such as poly-methyl-methacrylate (PMMA), are crazing and shear yielding. Crazing is formed because of the nucleation of micro-voids in the location of stress concentrations and shear yielding plastic deformation in the form of shear band.

A Phase field model based on Griffith’s theory is used to model the response of material under different loading condition ranging from pure deviatoric to isotropic volume expansion. The benefits of phase field modeling is that it can reduce the implementation complexity as it does not need to track the discontinuities in the displacement field. The model predictions for the macroscopic volumetric and deviatoric stress-strain response and phase field contour of PMMA are then compared with experimental data reported in
the literature and atomistic simulation’s results whose yielding criterion is energy-based and does not make assumption on whether the deformation is dominated by deviatoric strain or volumetric strain but the rate of mechanical work per unit volume. Our results shows that phase field model can the response of crazing behavior accurately in three dimensions. The outcome indicate that a 27% reduction of phase field damage parameter will achieved before the crazing emerges and the material yielding for any loading condition.
CHAPTER 1. INTRODUCTION

Glassy polymers play an important role in industry because many commercial products are manufactured from it. For instance, it is used to manufacture the matrix of composite used in the Dreamliner 787 as shown in figure 1-1. Unfortunately, because this kind of material is easy to fail in brittle manner under tension, it is timely to understand the failure mechanism of amorphous polymers. For amorphous polymers, there are two failure mechanisms. One is craze formation. Crazing is localized defects that contain micro-voids and fibrils. Another one is shear yielding which is plastic deformation in the form of shear band that may be localized for diffuse. When polymer material yielding in the form of crazing, it will be prefer brittle failure if the material have certain plasticity otherwise it will be present in the way of ductile failure if it has more viscoplastic deformation. When crazing is dominant, this mechanism is considered as precursor to brittle failure of material[1]. Unlike crazing, shear yielding is thought to cause ductile failure because fracture involves relatively large deformations[2]. In past decades, there are many attempts try to describe the deformation mechanism in polymers during the process of failure.
At microscopic scale level, Donald and Kramer [3][4] explored the kinetics of craze growth and first observed zones, which contained a large plastic deformation. Donald and Kramer[4] conclude the two effects that shear deformation on crazing. First one is shear deformation leads to oriented polymer area to serve as an access for craze propagation. Second one is that shear bands will lower the plastic stresses in front of the craze tips and slow down the process of craze propagation. Craze nucleation, growth and the other micromechanics of craze were reviewed in detail by Kramer [5]. Crazes are very similar to cracks as both of them have sharp planar surface[6]. But crazes have structure that is more complicated than cracks. Crazes contain micro voids and polymer fibrils that can carry the load of craze structure. Crazing propagation is basically divided into three steps: 1. Craze initiation, 2. Craze widening, and 3. Craze breakdown. However, the mechanisms behind these steps are still not clearly understood. For craze initiation, the mechanism has not clearly identified. Many criteria have been proposed at different length scale, which indicated that imitation of craze is a stress dependent phenomenon.
At macroscopic scale level, Sternstein and Ongchin[7] conducted experiments to observe crazing in pre-defined stress fields poly-methyl methacrylate (PMMA) samples. Both the stress field requirements for craze formation and shear yielding were studied in their macroscopic scale level experiments. However, due to the reason that both mechanisms could occur simultaneously, or one may precede the other, glassy polymer material would fail either craze formation or shear yielding. As concluded in another work of Ongchin[8], “the two forms of yielding in glassy PMMA have been characterized with respect to their general stress field dependences.” The propagation of craze could be expressed by a critical value of volumetric stress and for shear yielding, it can be best expressed by volumetric and deviatoric components of stress field. Also, in the study of Quinson et al.[9], shear yielding could be expressed by applied stress field of pressure modified Von Mises criterion. The experimental results at 20 °C of Quinson’s agreed with the ones from Bowden and Jukes [10] who conclude that pressure modified von Mises criterion more closely represents the macroscopic yielding behavior of PMMA.

Meanwhile, the strain invariant failure theory (SIFT) proposed by Gosse et al.[11] defines failure in terms of the maximum value of the volumetric and deviatoric strain invariants in contrast to other failure theories that define failure in terms of strength values. In this theory, the material fails when either the volumetric strain or the deviatoric strain reach a critical value.

The methodology used in this work is phase field damage model. Phase field model does not require numerical tracking of discontinuities in the displacement field[12]. Compared to models that using finite element methods in conjunction with Griffith’s linear elastic
fracture mechanics, this approach allows the fracture surface approximated by a phase field so that the craze boundary is smoothed over a small region. The Phase Field model, which couples plastic shear deformation and crazing, is used to solve onset yielding deformation for a family of loading conditions ranging from pure deviatoric to isotropic expansion. In dealing crazing mechanism during crazing voids nucleating and coalescing till the onset of fracture, the model use similar techniques that used to model fracture[13]. The results will be verified and modify in order to capture more accurate trend of shear deformation. Shear damage will be added based on classical plasticity models. The study will show that Phase Field model can be used to model crazing under onset yielding deformation for a wide range of loading conditions. Agreed with the one dimensional loading example in Miehe et al.[14] and Hughes et al.[12], one unique critical value of phase field damage parameter for any loading condition is obtained.
CHAPTER 2. YIELD CRITERIA

2.1. Introduction

In this chapter, we will go through three failure criteria that describe the mechanical response of glassy polymer. In section 2.2, we will discuss about the pressure modified von Mises failure criterion, which is dependent on both volumetric and deviatoric stress tensor. The failure mode of shear yielding can be best expressed by pressure modified von Mises failure criterion. In section 2.3, we will talk about another criterion, which is designated by volumetric stress tensor only, and the failure mode of crazing is expressed ideally by this criterion. Last but not at least, in section 2.4, we will talk about Strain Invariant Failure Theory (SIFT), which is a strain based criterion and is dependent on volumetric and deviatoric strain. SIFT has the potential to describe both glassy polymer failure mechanisms (shear yielding and crazing).

2.2. Shear Yielding: Pressure Modified Von Mises Failure Criteria

As mentioned previously, the dependences of volumetric stress are very different for crazing and shear yielding. For shear yielding, the failure mechanism could be expressed by applied stress field of pressure modified von Mises criterion.
\[ \sigma_{cr} = \sigma^d + \mu_{vM} \sigma^v \]  

(1)

In which \( \sigma^d \) is the deviatoric stress and \( \sigma^v \) is the volumetric stress. Both of them can be written in the form of principal stresses:

\[ \sigma^d = \sqrt{\frac{1}{2} [(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2]} \]  

(2)

\[ \sigma^v = \frac{(\sigma_1 + \sigma_2 + \sigma_3)}{3}. \]  

(3)

The parameter \( \sigma_{cr} \) is the critical yield stress and the pressure coefficient \( \mu_{vM} \) is a constant that quantify the yield stress sensitivity to volumetric stress. From another Sternstein’s study[7], \( \mu_{vM} \) is relatively insensitive to temperature. Conclude from Quinson’s experimental data, which was obtained under different stress states, confirm that the relationship between the critical yield stress and volumetric stress is linear. The experimental results at 20 °C of Quinson’s agreed with the ones from Bowden and Jukes [10] who conclude that pressure modified Von Mises criterion more closely represents the macroscopic shear yielding behavior of PMMA.

2.3. Crazing Failure Criteria

Different from shear yielding, as pointed out by Sternstein and Ongchin [8], crazing has been shown to obey the yielding criteria under biaxial stress state designated only by first stress invariant or we say volumetric stress, note that \( \sigma_3 \) is zero in the experiment so the expression of deviatoric stress is different from Eqn. (2):
\[ \sigma_1 \geq A + \frac{B}{\sigma_v} \quad (4) \]

\[ \sigma_i = \frac{|\sigma_1 - \sigma_2|}{\sqrt{2}}. \quad (5) \]

A and B can be expressed by Boltzmann’s constant and other experimental determined data.

\[ A(T) = A(0) \exp\left(\frac{Q_a}{kT}\right) \quad (6) \]

\[ B(T) = B(0) \exp\left(\frac{Q_b}{kT}\right). \quad (7) \]

Both of them are positive and are constants dependent on temperature. Tjissen et al. [15] using experimental data from Sternstein and Myers [16], \( A(0) = 0.253 \text{MPa} \) and \( B(0) = 4.402 \times 10^{-3} \text{MPa}^2 \), \( \frac{Q_a}{k} = 2322 \text{K} \) and \( \frac{Q_b}{k} = 4205 \text{K} \). The \( A(T) \) and \( B(T) \) at room temperature which is 20 °C is \( A=70 \text{ MPa} \) and \( B=7500 \text{ MPa}^2 \). Conclude from all these observations, the sufficient conditions needed to initiate a craze formation in uniaxial tension is only dependent on the hydrostatic pressure while in shear yielding it is depend on both the octahedral shear stress and the hydrostatic pressure. From all these macroscopic scale experiments conducted by Sternstein, Ongchin and Quinson, we have a picture about what parameters we need to consider when analysis the initiation criteria of yielding of amorphous polymers.
2.4. Strain Invariant Failure Theory

Strain invariant failure theory (SIFT) proposes that yielding occurs when either the volumetric strain or the deviatoric strain reach a critical value. Two strain invariants which represent dilatation and distortion respectively are defined follow Eqn. (8) and (9):

\[ \varepsilon^v = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 \]  

\[ \varepsilon^d = \sqrt{\frac{1}{2} \left[ (\varepsilon_1 - \varepsilon_2)^2 + (\varepsilon_2 - \varepsilon_3)^2 + (\varepsilon_3 - \varepsilon_1)^2 \right]} \]  

Even though, SIFT is strain based and pressure-modified von Mises criterion is stress based, if we convert \( \varepsilon^v \) and \( \varepsilon^d \) to \( \sigma^v \) and \( \sigma^d \) by multiply shear modulus and bulk modulus, we could find that there is a overlap and correlation between the pressure-modified von Mises criterion and the strain Invariant failure theory in figure 2-1. It is important to notice that the material assume to be elastic in SIFT so the failure boundary is horizontal and vertical line.
Figure 2-1: Deviatoric stress versus volumetric stress at failure.
CHAPTER 3. NUMERICAL MODELS

3.1. Introduction

In order to take the advantage of computational engineering development, several numerical models have been proposed to predict the mechanism of crazing using a fracture mechanics approach. In this chapter, we will talk about the numerical models, mainly cohesive zone model that try to simulate glassy polymer material. The basic idea of cohesive zone model is to regard the part in front of a sharp crack as crazing and when crazing opening reaches a critical width then the crazing get advanced. In the later part of section 3.2, we will also talk about a modification of cohesive surface model, which incorporate the plastic strain into the deformation rate, so that the model could capture more accurate response of yield softening which due to the shear yielding.

3.2. Cohesive Zone Model

Different scale level experiments about craze formation and shear yielding provide the solid basis for numerical simulations of failure analysis of amorphous glassy polymers. Experiments are based on two main different length scales.

For macromechanical level, high density of crazes initiated around structure defects[7][17] and for micromechanical level, craze widening and breakdown could be used to represent craze propagation. Many mechanical models at either micromechanical
scale or macromechanical scale level tried to explain the behavior of crazes have been proposed. There are some studies dealing crazing by a fracture mechanics approach which is originally by Doll et al.[18]. In this approach, craze loaded in Mode I and become a crack once the open width reaches its critical threshold value.

In order to predict craze formation and shear yielding using numerical methods, several researchers have developed the mechanics of crazing using a fracture mechanics approach. The advances in computational mechanics enhanced this trend and possibility. Doll[18] observed that the crack propagates when the opening of the zone reached a critical value and Williams[19] used a modified Dugdale model to represent a craze at a crack tip and let the crack propagate when the opening of it reached a critical value which Doll have observed. Basically, this approach let craze nucleates at the crack tip ahead of the crack. Plasticity increases as the craze extends under Mode I until the critical width of a craze reached and then the previous sharp crack evolves as a blunt crack.

Tijssens and coworkers[15] adopted this approach and a cohesive surface model for crazing in polymer is developed in a finite element method. The simulation is modelled by implanted high density cohesive surface into the continuum and the purpose of using finite element method is to discretize cohesive surface and continuum. Tijssens account finite strains in the continuum description to model the viscoelastic. The elasticity of the material is governed by hypoelastic relation in terms of the Second Piola-Kirchhoff stress and the Lagrangian strain. The traction separation law was used to model Craze initiation, widening and breakdown mechanisms. The traction-separation law for craze initiation criteria was modified from Sternstein [3] and it accounted for craze widening by a rate-
dependent equation from Tijssens et al.[15]. In this way, the initiation of craze is controlled by hydrostatic stress and cohesive surface normal traction. The craze widening stage simulated based on a rate-dependent viscoplastic formulation. The final part, craze breakdown occurs once the fibrils inside the craze reached the maximum extension. Tijssens also considered that crazes have quite complex structure as they contain long cylindrical fibrils of polymer material, which can carry some tangential load when it is widening. So the rate-dependent equation can account for the resistance against tangential load either. The finite element implementation is compared by the experimental results of Sternstein et al.[7]. The study shows that the model is qualitatively able to capture the temperature-dependence of the craze development.

Estevez et al.[6] used the cohesive surface method which proposed by Tijssens et al.[15] to model the competition between craze formation and shear yielding of mode I fracture in amorphous polymers. The modification based on Tijssens’ cohesive surface model is that the plastic strain is incorporated into the deformation rate. The response of the bulk depends on the material sensitivity of craze initiation. The material performs elastic behavior and craze initiate before it reach up to the yielding stress. After that, as the crazes are widening, the plasticity take place. The crazes advance till internal fibrils start to break down and the crack propagation begins. The constitutive equations used to model the behaviors of glassy matric is based on ideas from Boyce et al.[20] with modification from Wu and Van der Giessen[21]. In the model of Boyce et al, the rate of deformation is decomposed into elastic part and plastic part. The elastic part response is expressed by hypoelastic law. For plastic part, as under transition temperature $T_g$, which
amorphous polymer performed glassy, the material’s initial yielding and strain softening depend on conditions like pressure, strain rate and temperature. The material need to be stressed to overcome its intermolecular resistance to segment rotation. The intermolecular resistance was modeled as ideally plastic. For rate and temperature dependence, Boyce used an equivalent plastic shear rate expression derived from Argon[22], which is based on a double-kink model:

\[
\dot{\gamma}^p = \dot{\gamma}_0 \exp\left[-\frac{A_m s_0}{T}\left(1 - \left(\frac{\tau}{s_0}\right)^{\frac{1}{2}}\right)\right] \quad \text{with} \quad s_0 = \frac{0.077 \mu}{1 - \nu} \quad \text{and} \quad \tau = \sqrt{\frac{1}{2} \sigma^d \cdot \sigma^d}.
\]

(10)

\(\mu\) is the shear modulus and \(\nu\) is Poisson’s ratio. \(\dot{\gamma}_0\) and \(A_m\) are material parameters and \(T\) is the absolute temperature. \(\tau\) is the shear stress and \(\sigma^d\) is the deviatoric component of applied stress.

In order to incorporate pressure dependence, Boyce modified the athermal yield stress, \(s_0\) of the material when plastic straining happens and introduced the parameter \(\tilde{s}\), which dependent on pressure as well as the evolving athermal shear resistance \(s\):

\[
\tilde{s} = s + \alpha P.
\]

(11)

The plastic straining \(s\) evolves through

\[
\dot{s} = h\left(1 - \frac{s}{s_{ss}}\right)\dot{\gamma}^p.
\]

(12)

\(s\) is the current athermal deformation resistance of the material. \(\alpha\) is the pressure coefficient, \(P\) is the hydrostatic pressure, \(s_0\) is the upper yielding point and \(h\) is the
slope of the yield drop with respect to plastic strain, $s_{ss}$ is the value $s$ reaches at steady state. So the effective athermal shear resistance $\tilde{s}$ replace $s_0$ to provide the constitutive law for $\dot{\gamma}^p$ with the dependence of pressure, temperature, rate and strain softening:

$$\dot{\gamma}^p = \dot{\gamma}_0 \exp\left[-\frac{A_\sigma \tilde{s}}{T} \{1 - \left(\frac{T}{\tilde{s}}\right)^{5/6}\}\right].$$

(13)

And the plastic dissipation rate per unit volume is defined by

$$D = \bar{\sigma} : \dot{\varepsilon}^p = \sqrt{2} \tau \dot{\gamma}^p.$$

(14)

Through a parametric study, the effect of craze widening rate on material response is analyzed and the outcome is that when the craze widening rate is slow, the process of craze opening would be slow and the polymer material will tend to have more shear yielding rather than crazing. Estevez also pointed out that the competition between craze formation and shear yielding is very substantially important before crazes internal fibrils breakdown. When plastic shear deformation dominates, the craze length will be shorter because of the redistribution of stress field in front of the craze tip. And when crazing dominants, the location of craze breakdown will coincides with the one of imitation.
CHAPTER 4. A PHASE FIELD DESCRIPTION OF DAMAGE

4.1 Introduction
Phase field was originally developed to analyze the phase transformations in metals. This methodology could also be used to analyze dislocation dynamics\cite{23} and partial dislocations in metals\cite{24}. In this chapter, we will go step by step to introduce how to use phase field model to describe the damage of glassy polymer material. We also include section 4.4 to discuss each parameter’s influence to the results.

4.2 Phase Field Formulation
In the phase field formulation of brittle fracture the surface of the set of discrete cracks is replaced by a phase field, \( d(x) \in (0,1) \). The value of the phase field is equal to 1 away from the crack and equal to zero in the crack. Here, the phase field represents the damage introduced in the materials due to crazing, the phase field is equal to 1 when the craze developed into a crack and it is less than 1 when the craze can still ear strength. The surface opening is approximated by the phase field approach used by Miehe and Bourdin et al.\cite{12,14,25} in which based on Griffith’s theory of brittle fracture. The energy needed to create a unit surface area during fracture is the critical energy density \( G_{cr} \). The energy of the craze is

\[
W^{cr} = \int_{\Gamma} G_{cr} \, dx .
\]  \hspace{1cm} (15)
Following Griffith’s theory of brittle fracture, the energy needed to create a surface is equal to the surface energy density times the area. While $\Gamma$ represents a fracture surface area in fracture models, here it represents the surface of the voids created during crazing.

With the phase field approximation this expression is replaced by:

$$W^{cr} = \int_G G_{cr} \, dx = \int_V G_{cr} \phi(d) \, dx.$$  \quad (16)

The volume of the damaged region is represented by the functional:

$$\phi(d) = \frac{d^2}{2l_0^2} + \frac{l_0}{2} |\nabla d|^2.$$  \quad (17)

$l_0$ is a model parameter which control the width of the craze. Higher value of $l_0$ represents larger width of craze. To incorporate the loss of stiffness in the craze zone the strain energy density following Miehe et al.[14] as:

$$a[\varepsilon_{ij}, d] = g(d) a_0 (\varepsilon_{ij}) = g(d) \left( \frac{1}{2} \kappa \varepsilon^v \varepsilon^v + \mu \varepsilon_{ij} \varepsilon_{ij} \right).$$  \quad (18)

$\kappa$ is the bulk modulus, $\mu$ is the shear modulus, $g(d) = (1 - d)^2$, $\varepsilon^v = \varepsilon$, and $\varepsilon_{ij}^d = \varepsilon_{ij} - \frac{\varepsilon^v}{3} \delta_{ij}$

is the deviatoric strain tensor. The stress tensor is defined as:

$$\sigma_{ij} = \frac{\partial a[\varepsilon, d]}{\partial \varepsilon_{ij}} = (1 - d)^2 (\kappa \varepsilon^v \delta_{ij} + 2 \mu \varepsilon_{ij}^d).$$  \quad (19)

The force conjugate to the damage field is:
\[ f = -\frac{\partial a[\varepsilon,d]}{\partial d} = 2(1-d)a_0(\varepsilon). \]  

(20)

The energy dissipation due to the growth of the craze is

\[ \dot{W}^{cr}(d,d) = \int V G_{cr} \frac{\delta \phi(d)}{\delta d} \dot{d} dx \geq 0. \]  

(21)

This dissipation should be positive and therefore, the two following conditions need to be satisfied:

\[ \frac{\delta \phi(d)}{\delta d} \geq 0 \text{ and } \dot{d} \geq 0. \]  

(22)

In order to satisfy these local constraints in Eqn. (22) along with minimization of the energy rate:

\[ \dot{A}[\varepsilon, \dot{\varepsilon}, d, \dot{d}] = \int V \left( \frac{\partial a}{\partial \varepsilon_{ij}} \dot{\varepsilon} - f \dot{d} \right) dx \]  

(23)

Following Miehe et al.[14], we define the threshold function \( Y_{cr} \):

\[ Y_{cr} = f - G_{cr} \frac{\delta \phi(d)}{\delta d} \leq 0. \]  

(24)

The extended dissipation functional \( D[d,\dot{d},\lambda] \)

\[ D[d,\dot{d},\lambda] = \int V (f \dot{d} - \lambda Y_{cr}) dx. \]  

(25)
\( \lambda \) is a Kuhn-Tucker coefficient for the ordinary convex problem given by Equations (21) - (23)[26] with the extended Lagrangian:

\[
L(\varepsilon, \dot{\varepsilon}, d, \dot{d}) = \dot{A}(\varepsilon, \dot{\varepsilon}, d, \dot{d}) + D(d, \dot{d}, \lambda).
\]  

(26)

The constraints in Eqn. (22) are satisfied by the definition of the extended dissipation with

\[
W_{cr} = \text{sup}_{\lambda \geq 0} D(\lambda, d, \dot{d}) .
\]  

(27)

The variation of the extended Lagrangian with respect to the four variables gives the following Kuhn-Tucker conditions:

\[
\sigma_{ij,j} = 0 \\
\dot{d} = \lambda \geq 0 \\
Y_{cr} \leq 0 \\
\dot{d} \cdot Y_{cr} = 0.
\]  

(28)

Note that the first Equation (28) is the equilibrium equation and that condition Eqn. (22) is satisfied. During loading, when the rate of damage, \( \dot{d} \), is positive we have from the last Equation (28) with (20) and (24)

\[
G_{cr} \frac{\delta \phi(d)}{\delta d} = 2(1-d)a_0(\varepsilon).
\]  

(29)

A closed form solution can be obtained when \( d(x) \) is constant:

\[
d = \frac{a_0(\varepsilon)}{a_0(\varepsilon) + \frac{G_{cr}}{2l_0}}.
\]  

(30)
This solution satisfies that the damage field approaches one as the elastic strain energy increases. The values of the critical energy density, $G_c$, and the length parameter $l_0$ need to be determined, to this end we compare this model to atomistic simulations of failure of PMMA by Jaramillo et al.[27].

4.2.1. Homogeneous Deformation

In this section we study the homogeneous solution by ignoring special derivatives of the damage field. With this approximation we compare our model to the atomistic simulations by Jaramillo et al.[27] These simulations are carried out in a small domain where the deformation occurs over the whole sample and it is not limited to localized craze zones or shear bands as in experiments. Therefore, these simulations are a good benchmark to determine the surface energy density and the length parameter $l_0$. It is important to notice that for a homogeneous damage field both constants are coupled and we obtain the ratio $G_c / 2l_0$. The simulations are performed by applying a strain of the form:

$$
\varepsilon = \varepsilon_i(t) \begin{pmatrix}
1 & 0 & 0 \\
0 & \alpha & 0 \\
0 & 0 & \alpha
\end{pmatrix}.
$$

(31)

$\alpha \in [-0.5, 1]$ to take into account the effect of triaxiality. Figure 4-1 shows the evolution of the damage phase field value $d$ for different loading paths from Equation (30) with the parameters in Table 4-1 and

$$
a[\varepsilon_i, d] = g(d) \left[ \frac{1}{2} \kappa (1 + 2\alpha)^2 \varepsilon_i^2 + \frac{2}{3} \mu (1 - \alpha)^2 \varepsilon_i^2 \right].
$$

(32)
Table 4-1: Elastic constants and fitted parameters.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$G_{cr}/2l_0$</td>
<td>45 MPa</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>3235 MPa</td>
</tr>
<tr>
<td>$\mu$</td>
<td>1240 MPa</td>
</tr>
</tbody>
</table>

Figure 4-1: Phase field for the family of the deformation paths.

Figure 4-2 shows the volumetric stress versus the volumetric strain calculated with our model with the elastic constants and material parameters in Table 4-1 and the atomistic simulations[27] with strain rates of $3.75 \times 10^8$ 1/s as dashed lines for comparison. The volumetric stress is defined in Eqn. (3) and volumetric strain is defined in Eqn. (8).
Figure 4-3 shows a comparison of the deviatoric stress versus the deviatoric strain calculated with the phase field model and atomistic simulations where the deviatoric stress is defined in Eqn. (2) and deviatoric strain is defined in Eqn. (9).

Figure 4-2: Volumetric stress versus volumetric strain. Dashed lines are atomistic simulations and solid lines correspond to the current model.
Figure 4-3: Deviatoric stress versus deviatoric strain. Dashed lines are atomistic simulations and solid lines correspond to the current model.

Better agreement between our results and the atomistic simulations is found for the volumetric stress and strain. The phase field simulations show a drop in the deviatoric stress for $\alpha = -0.33$ and $\alpha = -0.5$ while the atomistic simulations do not. To take into account the shear yielding behavior in the following section, we incorporate plastic deformation in shear to the damage model.

4.3 Shear Yielding

The evolution of damage field is affected by shear and volumetric deformation but it is clear from figure 4-3 that phase field damage model does not capture shear deformation as well as the volumetric part. To take into account damage in shear, we add a term based on classical plasticity models. The elastic strain energy density can be expressed as
\begin{equation}
a(\varepsilon_{ij}, d, \gamma) = g(d) \left[ \frac{1}{2} \kappa \varepsilon^\gamma e^\gamma + \mu (\varepsilon^d_{ij} - \varepsilon^p_{ij})(\varepsilon^d_{ij} - \varepsilon^p_{ij}) \right].
\end{equation}

The plastic strain defined in terms of a new variable \(\gamma\) as

\begin{equation}
\varepsilon^p_{ij} = \gamma \frac{\varepsilon^d_{ij}}{\varepsilon^d_{eff}}.
\end{equation}

Therefore the stress components are

\begin{equation}
\sigma_{ij} = (1 - d)^2 [\kappa \varepsilon^\gamma \delta_{ij} + 2 \mu (\varepsilon^d_{ij} - \varepsilon^p_{ij})].
\end{equation}

To obtain the constitutive equations we follow the same procedure described in previous chapter. We define the energy rate:

\begin{equation}
\dot{A}[\varepsilon, \dot{\varepsilon}, d, \dot{d}, \gamma, \dot{\gamma}] = \int_V \left( \frac{\partial a}{\partial \varepsilon_{ij}} \dot{\varepsilon}_{ij} - f_d \dot{d} - f_\gamma \dot{\gamma} \right) dx.
\end{equation}

Threshold function for the shear strain as

\begin{equation}
Y = f_\gamma - \frac{\partial w^p}{\partial \gamma} \leq 0
\end{equation}

where

\begin{equation}
f_\gamma = - \frac{\partial a}{\partial \gamma} = \frac{4}{3} (1 - d)^2 \mu (1 - \gamma) \varepsilon^d_{eff}
\end{equation}

is force conjugate to the plastic deformation and the plastic work density is
\[ w^p = Y_0 \gamma + \frac{n Y_0 \gamma}{n + 1} (\frac{\gamma}{\gamma_0})^{\frac{n+1}{n}}. \] (39)

The extended Lagrangian

\[ L[\varepsilon, \dot{\varepsilon}, d, \dot{d}] = A[\varepsilon, \dot{\varepsilon}, d, \dot{d}] + D[d, \dot{d}, \lambda] + D_\gamma[\gamma, \dot{\gamma}, \theta] \] (40)

with

\[ D_\gamma[\gamma, \dot{\gamma}, \theta] = \int_V (f_\gamma \dot{\gamma} - \theta Y) dx. \] (41)

\( \theta \) is a Kuhn-Tucker coefficient, minimizing the extended Lagrangian in Equation 40 we obtain the following Kuhn-Tucker conditions:

\[ \sigma_{ij,j} = 0 \]
\[ \dot{d} \geq 0 \]
\[ Y_{cr} \leq 0 \]
\[ d \cdot Y_{cr} = 0 \] (42)
\[ \dot{\gamma} \geq 0 \]
\[ Y \leq 0 \]
\[ \dot{\gamma} \cdot Y = 0 \]

From the last two Equation (42) we have a threshold condition for \( \gamma \) given by

\[ \dot{\gamma} = 0 \quad \text{if} \quad \frac{4}{3} \mu g(d) \varepsilon^d - Y_0[1 + (\gamma/\gamma_0)^{1/n}] < 0 \]

\[ \dot{\gamma} > 0 \quad \text{if} \quad \frac{4}{3} \mu g(d) \varepsilon^d - Y_0[1 + (\gamma/\gamma_0)^{1/n}] = 0 \] (43)

When \( n=1 \) and \( \dot{\gamma} \geq 0, Y = 0 \), therefore
\[
\frac{4}{3} \mu g(d) \varepsilon^d - Y_0 = \frac{4}{3} \mu g(d) \varepsilon^d + \frac{Y_0}{\gamma_0}.
\]

(44)

And

\[
d = \frac{a_0(\varepsilon_{ij}, d, \gamma)}{a_0(\varepsilon_{ij}, d, \gamma) + \frac{G_c r}{2l_0}}.
\]

(45)

Figures 4-4 shows the deviatoric stress-strain curves with the Equations (42) with \( Y_0 = 42 \) MPa, \( n = 1 \) and \( \gamma_0 = 0.015 \).

\[
\sigma^d \quad [\text{MPa}]
\]

Figure 4-4: Deviatoric stress versus deviatoric strain. Dashed lines are atomistic simulations and solid lines correspond to the model with constitutive law for shear damage.
After added a shear damage parameter $\gamma$, the phase field $d$ is still monotonically increasing but now it can be expressed in two parts. As showed in figure 4-5 below, the red solid curve is the phase field of current model of same loading condition with shear damage parameter and the blue solid curve represents the shear damage parameter $\gamma$. For all four loading conditions, at first part, the current phase field increases in form of Eq. (30) as same as the previous model because the shear damage parameter $\gamma$ has not evolve yet. When the condition $\dot{\gamma} \approx 0$, $Y = 0$ satisfied, $\gamma$ starts to evolve as expressed in Eq. (44), the phase field in the form of Eq. (45) increases slower then previous model. Moreover, the more shear deformation the loading condition has, the slower phase field increase will be.

![Figure 4-5: Original damage phase field (dash red), current damage phase field (solid red) and shear damage parameter (solid blue) for loading condition (a): $\alpha=0$, (b): $\alpha=-0.16$ and (c): $\alpha=-0.33$ (d): $\alpha=-0.5$ with constitutive law with shear damage.](image-url)
Figure 4-5: Continued.
4.4 Influence of Parameters

We conducted a parameter study in order to have a better understanding of the three very important parameters that in the constitutive law of phase field model. One parameter is $G_c/2l_0$ in Eqn. (30) that couple the critical surface energy density and the length parameter $l_0$. It plays a very important role in controlling the homogenous response of the material. One is $Y_0$ in Eqn. (43), which control the shear damage yielding stress in the model. Last one is $\gamma_0$ in Eqn. (44), which eventually control the phase field damage parameter. In order to have some ideas about the influence of the parameters in the numerical model, 16 sets of parameters have been selected and listed in Table 4-2. The set (a-0) in Table 4-2 is used as a reference.
Table 4-2: The sets of parameters used in this study.

<table>
<thead>
<tr>
<th>Set</th>
<th>$G_{cr} / 2l_0$ (MPa)</th>
<th>$Y_0$ (MPa)</th>
<th>$\gamma_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>a-0</td>
<td></td>
<td></td>
<td>0.015</td>
</tr>
<tr>
<td>a-1</td>
<td>45</td>
<td>42</td>
<td>0.03</td>
</tr>
<tr>
<td>a-2</td>
<td></td>
<td></td>
<td>0.0075</td>
</tr>
<tr>
<td>b</td>
<td>5</td>
<td>42</td>
<td>0.015</td>
</tr>
<tr>
<td>c-0</td>
<td></td>
<td></td>
<td>0.015</td>
</tr>
<tr>
<td>c-1</td>
<td>65</td>
<td>42</td>
<td>0.03</td>
</tr>
<tr>
<td>c-2</td>
<td></td>
<td></td>
<td>0.0075</td>
</tr>
<tr>
<td>d-0</td>
<td></td>
<td></td>
<td>0.015</td>
</tr>
<tr>
<td>d-1</td>
<td>5</td>
<td>30</td>
<td>0.03</td>
</tr>
<tr>
<td>d-2</td>
<td></td>
<td></td>
<td>0.0075</td>
</tr>
<tr>
<td>e-0</td>
<td></td>
<td></td>
<td>0.015</td>
</tr>
<tr>
<td>e-1</td>
<td>45</td>
<td>30</td>
<td>0.03</td>
</tr>
<tr>
<td>e-2</td>
<td></td>
<td></td>
<td>0.0075</td>
</tr>
<tr>
<td>f-0</td>
<td></td>
<td></td>
<td>0.015</td>
</tr>
<tr>
<td>f-1</td>
<td>45</td>
<td>60</td>
<td>0.03</td>
</tr>
<tr>
<td>f-2</td>
<td></td>
<td></td>
<td>0.0075</td>
</tr>
</tbody>
</table>
4.4.1. Influence of $G_{cr} / 2l_0$

According to Eqn. (43), phase field parameter $d$ is governed by strain energy $a_0(\epsilon, \gamma)$ and $G_{cr} / 2l_0$. Three different values of $G_{cr} / 2l_0$ (set (a-0, 1, and 2), set (b) and set (c-0, 1 and 2) in Table 4-2 are sufficient to let us have an understanding of its influence. As shown in table 4-3, the general differences between set (a-0), set (b) and (c-0) is in the value of $G_{cr} / 2l_0$. Set (a-0) has $G_{cr} / 2l_0$ equal to 45 MPa, set (b)’s $G_{cr} / 2l_0$ equals to 5 MPa and set (c-0)’s $G_{cr} / 2l_0$ equal to 65 MPa. In either case, the value of $Y_0$ equals 42 MPa and the value of $\gamma_0$ equals 0.015.

Table 4-3: Parameter sets for influence of $G_{cr} / 2l_0$.

<table>
<thead>
<tr>
<th>Set</th>
<th>$G_{cr} / 2l_0$ (MPa)</th>
<th>$Y_0$ (MPa)</th>
<th>$\gamma_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>a-0</td>
<td>45</td>
<td>42</td>
<td>0.015</td>
</tr>
<tr>
<td>b</td>
<td>5</td>
<td>42</td>
<td>0.015</td>
</tr>
<tr>
<td>c-0</td>
<td>65</td>
<td>42</td>
<td>0.015</td>
</tr>
</tbody>
</table>
Figure 4-6: Influence of parameters [set (a-0), (b) and (c-0)].
Figure 4-6-b shows the deviatoric stress-strain curve of set (b) and figure 4-6-c-0 show the one of set (c-0). Compared to figure 4-6-a-0, which is the reference set, it can be seen that higher value of $G_{cr} / 2l_0$ will lead to a higher value of yield stress and yield strain which means the material become harder when $G_{cr} / 2l_0$ get higher. The reason is because as we couple the critical density energy $G_{cr}$ and length parameter $l_0$ together, if the critical density energy is constant, then higher value of $G_{cr} / 2l_0$ means lower value of $l_0$ and lower value of $l_0$ means the width of craze is smaller and the material itself is less damaged. It also need to be pay attention that for loading conditions with $\alpha$ equals to -0.16, -0.33 and -0.5, when the value of $G_{cr} / 2l_0$ is relatively small, the shear parameter $\gamma$ does not even evolve, which is not correct according to the experimental observation. We will discuss more about it in next two sections.

4.4.2. Influence of $Y_0$

According to Eqn. (42), the shear damage parameter $\gamma$ is governed by $Y_0$. Two sets of $Y_0$ (set (e-0) and (f-0) in Table 2) could give us the idea of its influence. The difference between set (e-0) and (f-0) is only in the value of $Y_0$. Set (e-0) has $Y_0$ equal to 30 MPa and set (f-0)’s $Y_0$ equals to 50 MPa. In either case, the value of $G_{cr} / 2l_0$ equals 45 MPa and the value of $\gamma_0$ equals 0.015.
Table 1-4: Parameter set for influence of $Y_0$.

<table>
<thead>
<tr>
<th>Set</th>
<th>$G_{cr}/2l_0$ (MPa)</th>
<th>$Y_0$ (MPa)</th>
<th>$\gamma_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>a-0</td>
<td>45</td>
<td>42</td>
<td>0.015</td>
</tr>
<tr>
<td>e-0</td>
<td>45</td>
<td>30</td>
<td>0.015</td>
</tr>
<tr>
<td>f-0</td>
<td>45</td>
<td>60</td>
<td>0.015</td>
</tr>
</tbody>
</table>

Figure 4-7: Influence of parameters [set (e-0) and (f-0)].
Figure 4-7-e-0 shows the deviatoric stress-strain curve of set (e-0) and figure 4-7-f-0 show the one of set (f-0). Compared to the reference set (a-0)’s deviatoric stress-strain curve, it is clear that higher value of $Y_0$ will lead to a higher value of yield stress and yield strain (plastic shear deformation). The reason is because according to Eqn. (41), the value of deviatoric strain equals to $3Y_0/4\mu g(d)$. So the choice of $Y_0$ will influence when the plastic shear deformation starts or in other word, when the shear damage parameter $\gamma$ start to evolve.

4.4.3 Influence of $\gamma$

As mentioned above, from figure 4-6-b we can see that the shear damage parameter $\gamma$ does not even evolve under the condition of set (b). The influence of $\gamma_0$ need to be analyzed. Three different values of $\gamma_0$ (set (d-0), (d-1) and (d-2) in Table 4-5 are sufficient to let us have an understanding of its influence. The general differences between set (d-0), (d-1) and (d-2) is in the value of $\gamma_0$. Set (d-0) has $\gamma_0$ equal to 0.015, set (d-1)’s $\gamma_0$ equals to 0.03 and set (d-2)’s $\gamma_0$ equal to 0.0075. In either case, the value of $G_{cr}/2l_0$ equals 5 MPa and the value of $Y_0$ equals 30 MPa.

<table>
<thead>
<tr>
<th>Set</th>
<th>$G_{cr}/2l_0$ (MPa)</th>
<th>$Y_0$ (MPa)</th>
<th>$\gamma_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>d-0</td>
<td>5</td>
<td>30</td>
<td>0.015</td>
</tr>
<tr>
<td>d-1</td>
<td>5</td>
<td>30</td>
<td>0.03</td>
</tr>
<tr>
<td>d-2</td>
<td></td>
<td></td>
<td>0.0075</td>
</tr>
</tbody>
</table>
Figure 4-8: Influence of parameters [set (d-0), (d-1) and (d-2)].
From figure 4-8, it can be seen that the value of $\gamma_0$ will change the shape of deviatoric stress-strain curve after the plastic shear deformation. Smaller value of $\gamma_0$ leads to a higher value of yield stress.

In order to have a better understanding of the relationship between $\gamma$ and, figure 4-9 is included for illustration. According to figure 4-9 below, smaller value of $\gamma_0$ will lead to a smaller value of $\gamma$ when the other parameters’ value are fixed. It is because according to Eqn. (43), phase field damage parameter $d$ is a function of $\gamma$ and lower value of $\gamma$ will leads to less plastic shear deformation.

Figure 4-9: Original damage phase field (dash red), current damage phase field (solid red) and shear damage parameter (solid blue) for loading condition $\alpha=-0.33$ of set (d-0), (d-1) and (d-2).
Figure 4-9: Continued.
CHAPTER 5. RESULTS

5.1. Introduction

In this chapter, we will validate our results calculated using phase field model by comparing to other experimental and simulation results from other literature reports.

5.2. Yield Stress Results

The validity of the yield criterion for craze formation and shear yielding were determined in experiments with different loading conditions and geometries. In order to validate our model, we compare our results with the ones from Sternstein’s [7], Quinson et al. [9] and Jaramillo et al. [26]. While in Sternstein’s work the yield is considered to be the maximum in the stress-strain curve. However, in some experiments such maximum is not found. Quinson’s defines the yield stress as the stress corresponding to the onset of plastic deformation. This stress is determined via residual strain measurements after unloading. In the work of Jaramillo et al.[27], they define the yield strain and stress based on the rate of mechanical work and the yield point is defined where the maximum mechanical work at constant strain rate is reached:
\[ \dot{W} = \frac{1}{V_0} \int_V \sigma_i \dot{\varepsilon}_i \, dx. \] 

(44)

Figure 5-1: Mechanical work performed per unit volume and time for the family of the deformation paths explored. The Maximum of these curves define the yield condition. Dashed lines are atomistic simulations and solid lines correspond to the current model. The loading family is separated into positive loading condition and negative loading condition.
Figure 5-1: Continued.

Figure 5-1 shows the mechanical work at constant strain rate and the various loading conditions. Using the same yield definition, the pattern of the current model and atomistic simulation is very similar. The mechanical work for all case increases with time early in the deformation process. The onset of yielding is defined as the condition of maximum mechanical work rate at constant strain rate. This condition applied to the current model yields
\[
\dot{W} = \frac{1}{V_0} \int (1-d)^2 (\kappa \varepsilon^\gamma \delta_y + 2 \mu \varepsilon_y^d) \dot{\varepsilon} dx
\]

\[
= V(\alpha, \varepsilon_1) \cdot \sigma(\varepsilon_1) = \frac{V(\alpha, \varepsilon_1)}{V_0} (1 - \frac{1}{G_c}) (2\sigma_0(\varepsilon) \dot{\varepsilon}_1) \varepsilon_1
\]

(45)

Figure 5-2: Pressure-modified von Mises plot (deviatoric stress at yield vs. pressure) including Phase Field calculations (Red), atomistic simulations (Blue) and experiments (Green, Yellow, Orange and Brown); Part (b) is part of Part (a) between \( \sigma^v \in [-50,65] \) MPa.

Figure 5-2 shows the deviatoric stress as a function of pressure at the yield point for the various loading conditions. The atomistic simulation results (blue dashed line) which are
obtained by yield criteria based on the rate of mechanical work and experimental data (green dashed line) which can be characterized by pressure modified von Mises criteria both show a linear decrease in deviatoric stress at the yield point with decreasing pressure and our yield points which are obtained by the same definition of Jaramillo et al.[27]’s energy-based mechanical work and we can get the similar results by only adjusting the value of $G_{cr}/2l_0$. For instance, in figure 10 above, with $G_{cr}/2l_0$ equal to 45 MPa, we could get a linear relationship between deviatoric stress and pressure with a very similar slope value.

Figure 5-3: Deviatoric (Blue), volumetric (Red) stress and critical stress (Green) as a function of transverse to longitudinal ratio. Dashed lines are atomistic simulations and solid lines correspond to the current model.

Figure 5-3 shows the deviatoric, volumetric and critical stress as expressed in Eq. (1) at the yield point as a function of the loading condition. The deviatoric stress decreases from around 178 MPa to 0 and volumetric stress increases from 0 to nearly 177 MPa
while the loading condition increases from -0.5 to 1. The critical yield stress first increases from 178 MPa to 200 MPa then decreases to roughly 97 MPa. For comparison, atomistic simulation results also gives the similar pattern.

In order to find the analytical critical strain $\varepsilon_{1cr}$, we used the following process. The expression of the derivation of mechanical work rate respect to strain is showed as below:

$$
\frac{dW}{d\varepsilon_i} = \frac{\partial V(\alpha, \varepsilon_i)}{\partial \varepsilon_i} \cdot \sigma(\varepsilon_i) + \frac{\partial \sigma(\varepsilon_i)}{\partial \varepsilon_i} \cdot V(\alpha, \varepsilon_i)
$$

$$
= 2a_0(\varepsilon_i)G_{cr}^2 \dot{\varepsilon}_i \{G_{cr}[1 + (2 + 4\alpha)\varepsilon_i] - 2a_0(\varepsilon_i)l_0 \varepsilon_i^2 [3 + (2 + 4\alpha)\varepsilon_i]\}
\frac{1}{(G_{cr} + 2a_0(\varepsilon_i)l_0 \varepsilon_i^2)^3}
$$

and

$$
\varepsilon_{1cr} = \frac{1}{6(1 + 2\alpha)} \left\{-3 + \frac{3^{2/3}[-3a_0l_0^3 - 2G_{cr}(1 + 2\alpha)^2]}{[9a_0^3l_0^3 + \sqrt[3]{3a_0^3l_0^3[27a_0^3l_0^3 - (3a_0l_0 + 2G_{cr}(1 + 2\alpha)^2)^3]]^{1/3}}
\right.

- \left.\frac{3^{1/3}[9a_0^3l_0^3 + \sqrt[3]{3a_0^3l_0^3[27a_0^3l_0^3 - (3a_0l_0 + 2G_{cr}(1 + 2\alpha)^2)^3]]^{1/3}}{a_0l_0}\right\}
$$

Set derivation equal to zero and solve for critical strain. Because the model include the modified constitutive law for shear damage, it is able to capture more accurate trend of the response of PMMA. As depicted in figure 5-4, we found out that although the value of the critical strain depends on the loading condition but the damage parameter at failure is always close to a constant with any loading condition. It is in agreement with the one dimensional loading example in Miehe and Hughes if we substitute (47) into (32), (30)
and (43) we obtain a series of data points close to a unique critical value of the damage parameter for any loading condition as shown in figure 5-4.

Figure 5-4: Deviatoric (Blue), volumetric (Red) strain and critical phase filed value (Green) as a function of transverse to longitudinal ratio. Dashed lines are atomistic simulations and solid lines correspond to the current model.
CHAPTER 6. CONCLUSION

In this work, we have extended the phase field model which Miehe used to solve quasi-static brittle fracture problem to characterize the yielding condition of the amorphous PMMA crazing and shear yielding problem under a wide range of loading conditions including pure deviatoric to isotropic volume expansion. The phase field method not only removes the requirement of numerically track displacement discontinuities and but also represent craze smoothly. In this study, we have conducted numerical experiments for crazing propagation, shear yielding and branching of entire loading family. The input parameters needed to model the PMMA crazing within the phase field model include the elastic constants, the constant $G_c$ which scales the work dissipated during crazing and length scale parameter $l_0$ which control the width of the smooth approximation of the craze and the shear damage equation (Eq. 39). All plots have indicated that phase field model can the response of crazing and shear yielding behavior accurately. Not only agreed with the results from Jaramillo’s work that the simulation results indicated that yield occurs when either the volumetric or deviatoric strains reach a critical value but more importantly, we found out that yield occurs when phase field damage parameter reaches a critical constant for any loading condition which means the critical value of
phase field is independent of material parameters. And this outcome indicate that phase field damage parameter will reach 0.27 before the crazing emerges and the material yielding. It has been shown in this study that Phase field formulation can be used to simulate the shear yielding and crazing and capture relatively accurate homogeneous response of the damage-elastic model. We believe that this formulation can be extended and be used to conduct numerical simulation for craze propagation and breakdown in two and three dimensions. It is shown in this study that the capability of phase field formulation can accommodate such study.
LIST OF REFERENCES


APPENDIX: CODE OF PHASE FIELD MODEL

#include <stdio.h>
#include <math.h>
#define young 3300     /*young's modulus*/
#define nu 0.33         /*poisson ratio*/
#define k 3235.2941    /*Bulk modulus={young/3/(1-2*nu)}*/
#define mu 1240.6015    /*Shear modulus={young/2/(1+nu)}*/
#define gc 45           /*Gc over 2l*/
#define n 1             /*Hardening factor*/
#define Y 42            /*gamma relavent variable*/
#define g0 0.015        /*gamma relavent variable*/
#define xmin 0  /*initial strain*/

#define xstep 0.001 /*strain step*/

#define ggmin 0

#define ggstep 0.00001

#define alpha -0.5  /*---LOADING CONDITION (1, 0.5, 0.25, 0, -0.16, -0.33, -0.5)---*/

int main()
{

double x[401],dtest[401],gtest[401],d[401],g[401],tem[401],temp[1001],diff[1001];
double ev[401],sv[401],ed[401],sd[401],w[401];
double root[4],droot[4];
int x1, x2, x3, x4;
int x3i;
int i,p;
int j = 0, q = 0, m = 0;

double dd[100001], gamma[100001], gg[100001], dsub[100001], G[100001], glast;

double allg[400][100];

/*-----For test (d & g)-----*/

for (i = 0; i < 401; i++)
{
    x[i] = xmin + i * xstep; /*Applied strain*/

    dtest[i] = 1.00 / (1.00 + gc / (0.5 * k * x[i] * x[i] * (1 + 2.0 * alpha) * (1 + 2.0 * alpha) + 2.0 * mu / 3.0 * x[i] * (1.0 - alpha) * x[i] * (1.0 - alpha))); /*d - (phase_field) test*/

    gtest[i] = Y - (4 * mu / 3 * (1 - dtest[i]) * (1 - dtest[i]) * x[i] * (1 - alpha));

    // gtest[i] = (4 * mu / 3 * (1 - dtest[i]) * (1 - dtest[i]) * x[i] * (1 - alpha)) * (Y / 4 * mu / 3 * (1 - dtest[i]) * (1 - dtest[i]) * x[i] * (1 - alpha) + Y / g0); /*gamma test*/
}

/*-----Find 4 roots-----*/

for (i = 0; i < 400; i++)
{

if ((gtest[i]*gtest[i+1])<0)
{
    root[j] = x[i];
    root[j+1] = x[i+1];
    x3i = i;
    j = j+2;
}
if (j==5)
    break;
}

x1 = root[0]; /*1st point before 1st root */
x2 = root[1]; /*2nd point after 2st root */
x3 = root[2]; /*1st point before 1st root */
x4 = root[3]; /*2nd point after 2st root */

printf("%f %f %f %f \n", root[0], root[1], root[2], root[3]);
j=0;
for (i = 0; i <= 400; i++)
{

    /*-----Condition I-----*/

    if (x[i] >= 0 && x[i] <= root[0])
    {
        d[i] = 1 / (1 + gc / (0.5 * k * x[i] * x[i] * (1 + 2 * alpha) * (1 + 2 * alpha) + 2 * mu / 3 * (x[i] * (1 + 2 * alpha)) * (x[i] * (1 - alpha)))); /*d1 phase field-1*/

        sd[i] = 2 * mu * (1 - d[i]) * (1 - d[i]) * x[i] * (1 - alpha); /*sd1 deviatoric stress-1*/

        w[i] = (1 - d[i]) * (1 - d[i]) * (k * (1 + 2 * alpha) * (1 + 2 * alpha) * x[i] + 2 * mu * (x[i] * (1 - alpha) - 0)) * (1 - alpha) * (1 + x[i] * (1 + 2 * alpha)); /*w1 work-1*/
    }

    /*-----Condition II-----*/

    else if (x[i] >= root[1] && x[i] <= root[2])
    {
        // Code for Condition II
    }
}
j=0;

for ( p =0; p<100001;p++)
{

gg[p] = ggmin+p*ggstep;

gg[p+1]=ggmin+(p+1)*ggstep;

dsub[p]=(1/(1 + gc/(0.5*k*x[i]*x[i]*(1 + 2*alpha)*(1 + 2*alpha) + 2*mu/3 *((1 - alpha)*x[i] - gg[p])*((1 - alpha)*x[i] - gg[p]))));

dsub[p+1]=(1/(1 + gc/(0.5*k*x[i]*x[i]*(1 + 2*alpha)*(1 + 2*alpha) + 2*mu/3 *((1 - alpha)*x[i] - gg[p+1])*((1 - alpha)*x[i] - gg[p+1]))));

G[p]=(4*mu/3*(1-dsub[p])*(1-dsub[p])*x[i]*(1-alpha))*gg[p]+Y*pow(g0,-(1.0/n))*pow(gg[p],(1.0/n))+Y-(4*mu/3*(1-dsub[p])*(1-dsub[p]))*x[i]*(1-alpha);
\[
G[p+1] = (4*\mu/3*(1-d_{sub}[p+1])*(1-d_{sub}[p+1])*x[i]*(1-alpha) + Y*\text{pow}(g0,-(1.0/n))*\text{pow}(gg[p+1],(1.0/n))+Y-(4*\mu/3*(1-d_{sub}[p+1])*(1-d_{sub}[p+1])*x[i]*(1-alpha)) \\
//\gamma[p] = (4*\mu /3*(1 - d[p])*(1 - d[p])* x[i]*(1 - alpha) - Y)/(Y/g0 + 4*\mu/3*(1 - d[p])*(1 - d[p])* x[i]*(1 - alpha)); \\
//\gamma[p+1] = (4*\mu /3*(1 - d[p+1])*(1 - d[p+1])* x[i]*(1 - alpha) - Y)/(Y/g0 + 4*\mu/3*(1 - d[p+1])*(1 - d[p+1])* x[i]*(1 - alpha)); \\
//\text{diff}[p] = 1/(1 + gc/(0.5*k*x[i]*x[i]*(1 + 2*alpha) + 2*mu/3 *((1-alpha)*x[i]-\gamma[p])*((1-alpha)*x[i]-\gamma[p]))))-d[p]; \\
//\text{diff}[p+1] = 1/(1 + gc/(0.5*k*x[i]*x[i]*(1 + 2*alpha) + 2*mu/3 *((1-alpha)*x[i]-\gamma[p+1])*((1-alpha)*x[i]-\gamma[p+1]))))-d[p+1]; \\
//if (\text{diff}[p]<0 && \text{diff}[p+1]>0) \\
\text{if (G[p]*G[p+1]<0) \\
\{ \\
\text{g[i] = gg[p+1]; /*d2 phase field-2*/}
\}
if (g[i]-g[i-1]<0) g[i]=g[i-1];

allg[i][j] = g[i];

//break;

//printf("%f %f %f %f %f %f %f %d\n", x[i], dd[p],

diff[p], gamma[p], dd[p+1], diff[p+1], gamma[p+1], p);

//p = 1001;

j++;

}

//g[i]=(4*mu /3*(1 - d[i])*(1 - d[i])* x[i]*(1 - alpha) - Y)/(Y/g0 +

4*mu/3*(1 - d[i])*(1 - d[i])* x[i]*(1 - alpha)); /*gamma only in condition II*/

d[i]=(1/(1 + gc/(0.5*k*x[i]*x[i]*(1 + 2*alpha)*(1 + 2*alpha) + 2*mu/3

*((1-alpha)*x[i]-g[i])*((1-alpha)*x[i]-g[i]))));
\[ sd[i] = 2 \mu (1 - d[i])^2 (1 - x[i]) (1 - \alpha) g[i]; /*sd2 deviatomic stress-2*/ \]

\[ w[i] = (1 - d[i])^2 (1 - x[i]) (1 - \alpha) (1 + 2 \alpha) x[i] + 2 \mu (x[i] (1 - \alpha) g[i]) (1 - \alpha) (1 + x[i] (1 + 2 \alpha)); /*w2 work-2*/ \]

\[ glast = g[i]; \]

\[ \text{printf("allg: ");} \]

\[ \text{for (m = 0; m < j; m++)} \}

\[ \text{printf("%f", allg[i][m]);} \]

\[ \text{printf("\n");} \]

\[ \text{else if (x[i] >= root[3] && x[i] <= 0.4)} \]

\[ /*-----Condition III-----*/ \]
\[
\{ \\
\text{g}[i] = \text{glast}; \\
\text{d}[i] = 1/(1 + gc/(0.5k*x[i]*x[i]*(1+2*alpha)*(1+2*alpha)+2*mu/3*(x[i]*(1 - \alpha) - \text{glast})*(x[i]*(1 - \alpha) - \text{glast}))); /*d3 phase field-3*/ \\
//\text{d}[i] == 0; \\
\text{sd}[i] = 2*mu*(1 - \text{d}[i])*(1 - \text{d}[i])*(x[i]*(1 - \alpha) - \text{glast}); /*sd3 deviatoric stress-3*/ \\
\text{w}[i] = (1 - \text{d}[i])*(1 - \text{d}[i])*(k*(1+2*alpha)*(1+2*alpha)*x[i]+2*mu*(x[i]*(1 - \alpha) - \text{glast})*(1 - \alpha))*(1 + x[i]*(1+2*alpha)); /*w3 work-3*/ \\
\}
\]

/*-----variables that won't change expressions-----*/

\text{ev}[i] = (1+2*alpha)*x[i]; /*ev1=ev2=ev3 volumetric strain-1, 2, 3*/

\text{ed}[i] = (1 - \alpha)*x[i]; /*ed1=ed2=ed3 deviatoric strain-1, 2, 3*/
sv[i]=x[i]*(1+2*alpha)*k*(1-d[i])*(1-d[i]); /*sv1=sv2=sv3  volumetric
stress-1, 2, 3*/

FILE *f1 = fopen("PFMS_coupled_data.txt", "w");

if (f1 == NULL)
{
    printf("Error opening file!\n")
    exit(1);
}

/* print text */

//const char *text1 = "g,x,d,ev,sv,ed,sd,w";
/fprintf(f1, "\n", text1);

/* print integers and floats */

for (i = 0; i<=400; i++)
{
    fprintf(f1,
            "%f,%f,%f,%f,%f,%f,%f,%f\n",
            g[i], x[i], d[i], ev[i], sv[i], ed[i], sd[i], w[i]);
}

fclose(f1);

return 0;