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Dynamic Crack Initiation Toughness: Experiments and Peridynamic Modeling

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John T. Foster

Abstract

This is a dissertation on research conducted studying the dynamic crack initiation toughness of a 4340 steel. Researchers have been conducting experimental testing of dynamic crack initiation toughness, K_{Ic} , for many years, using many experimental techniques with vastly different trends in the results when reporting K_{Ic} as a function of loading rate. The dissertation describes a novel experimental technique for measuring K_{Ic} in metals using the Kolsky bar. The method borrows from improvements made in recent years in traditional Kolsky bar testing by using pulse shaping techniques to ensure a constant loading rate applied to the sample before crack initiation. Dynamic crack initiation measurements were reported on a 4340 steel at two different loading rates. The steel was shown to exhibit a rate dependence, with the recorded values of K_{Ic} being much higher at the higher loading rate. Using the knowledge of this rate dependence as a motivation in attempting to model the fracture events, a viscoplastic constitutive model was implemented into a peridynamic computational mechanics code. Peridynamics is a newly developed theory in solid mechanics that replaces the classical partial differential equations of motion with integral-differential equations which do not require the existence of spacial derivatives in the displacement field. This allows for the straightforward modeling of unguided crack initiation and growth. To date, peridynamic implementations have used severely restricted constitutive models. This research represents the first implementation of a complex material model and its validation. After showing results comparing deformations to experimental Taylor anvil impact for the viscoplastic material model, a novel failure criterion is introduced to model the dynamic crack initiation toughness experiments. The failure model is based on an energy criterion and uses the K_{Ic} values recorded experimentally as an input. The failure model is then validated against one class of problems showing good agreement with experimental results.

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Preface

This document is a reproduction of a Ph.D. dissertation submitted to the faculty of Purdue University. It has been reformatted here as a SAND report for archival within Sandia National Laboratories.

The focus of the research in this dissertation is separated into two main areas, experiments and numerical simulation. Each of the first two chapters, Introduction and Literature Review, will be divided into two main sections, separately describing each of these areas. Chapter 3 describes, in detail, the experimental procedure for measuring dynamic crack initiation at high loading rates and reports a selection of data for 4340 steel. Chapter 4 describes the theory and numerical implementation of a viscoplastic material model into a computational mechanics code using the peridynamic theory of solid mechanics. Chapter 5 describes a novel energy based failure criterion, its numerical implementation, and a selection of simulations and comparisons to experimental results. The final chapter summarizes the accomplishments of this research and gives suggestions for further investigation.

1 Introduction

1.1 Dynamic Fracture

Failure of engineering materials has been at the forefront of research for scientists and engineers for centuries. The pioneering work of Griffith [24] during the first part of the 20th century steered material failure research towards a crack-dominated analysis and the field of fracture mechanics was born. Irwin's [30, 31] work introduced us to the idea that the stress field near a crack could be modeled in a linear elastic fashion with only a small plastic zone near the crack tip. This idea of small scale yielding led to a parameter that could be used to describe the state of stress near the crack tip, called the stress intensity factor, K , with units of stress times square root of length, typically given in $\text{MPa}\sqrt{\text{m}}$ or $\text{ksi}\sqrt{\text{in}}$.

The rest of the 20th century was filled with subsequent analysis of crack tip stress and initiation, mostly formulated within this framework of linear elastic fracture mechanics (LEFM). Many parameters such as strain energy release rate, the J -integral [51, 54], and crack tip opening displacement (CTOD) have been related to the stress intensity factor. These many forms of analysis allowed experimentalists freedom and creativity in designing experiments to determine a crack's stress intensity factor. It was discovered through this experimentation that there is a limiting value of stress intensity factor that when exceeded will cause a crack to grow. This limiting value is called the fracture toughness and denoted by K_c . A material's fracture toughness is considered a material property, meaning it is constant irrespective of sample size or geometry. It is typically presented with respect to the opening mode of the crack as K_{Ic} , K_{IIc} , or K_{IIIc} . Figure 1.1 illustrates these opening modes.

In 1970 the American Society for Testing and Materials (ASTM) International published the original standard for finding the linear-elastic plane-strain fracture toughness, K_{Ic} , for metallic materials [29]. This standard is designated E 399 and the current revision at the time of this writing is 2006. ASTM has also developed standards for finding the fracture toughness for other types of engineering materials such as ceramics and polymers. All of these well defined procedures are only valid for quasi-static loading rates.

High-rate loads are encountered in many engineering applications and it is important to understand how these loading regimes affect the fundamental fracture mechanisms in order to assure the integrity of the material. Generally, high-rate loading is defined by the

Figure 1.1: Crack opening modes.

Figure 1.2: Single-edge notched specimen.

need to analyze the stress wave propagation in a material to fully understand its behavior. This stress wave phenomenon's action on crack propagation can be easily illustrated with an example taken abridged from Ravi-Chandar[49]: consider a single-edge notched specimen illustrated in Figure 1.2, let the load be applied by a tup, falling at a speed v and impacting on the specimen. The impact generates a stress wave that travels into the specimen, interacts with the crack and reflects from the far end. If the impact speed is sufficiently high, it is possible to initiate the fracture event before the arrival of the stress wave at the supporting posts. If the crack does not initiate upon the first pass of the stress wave, the wave will subsequently reflect between the top and bottom surfaces of the specimen and eventually put the beam into oscillatory motion. If the stress wave build up causes fracture to occur after the sample has obtained a dynamic equilibrium state, then this situation is analogous to the quasi-static regime and analysis can proceed according to the laws of elastostatics. It should be obvious that if the crack propagates with the first pass of the stress wave then a more complex analysis is needed. These types of crack initiation and propagation events where stress waves must be taken into consideration fall into the realm of *dynamic fracture mechanics*.

As with LEFM in the quasi-static regime, the literature on the subject of dynamic fracture is vast. There have been many analytic, numerical, and experimental investigations

in the area. Under high-rate loading the stress intensity factor is used as the near crack tip stress field characterization, but is called the dynamic stress intensity factor, $K(t)$, as it carries a time-dependence. Dynamic fracture criterion is typically separated into three parts *crack initiation*, *crack growth*, and *crack arrest* and each criterion is imposed independently on a growing crack. Corresponding to each criterion, dynamic crack initiation toughness, dynamic crack growth toughness, and dynamic crack arrest toughness are defined as material properties.

Dynamic crack initiation toughness is similar to the quasi-static fracture toughness in that it is the critical value of the dynamic stress intensity factor that when exceeded will cause a crack to start propagating. The dynamic crack initiation toughness is postulated as a function of both temperature and loading rate, $K_c(\dot{K}, T)$, where the loading rate, $\dot{K}$, is the time derivative of stress intensity factor. The temperature dependence, T , is noticed as a change in ductility from explicitly heating or cooling the sample and/or adiabatic heat generated from the inelastic deformation at the crack tip. The rate dependence most likely arises from the inelastic material response at the crack tip or the inertial nature of the stress field development near the crack tip process zone. The crack tip process zone, also called the crack tip plastic zone, is the area around the crack tip where inelastic processes occur influencing the initiation and growth of a crack. These inelastic processes could be dislocations, void nucleation, microcrack coalescence, etc. The whole field of LEFM is built on the idea of small scale yielding, this concept, while somewhat abstract, refers to the idea that if the crack tip process zone is “small” relative to the crack length, then K_c will adequately describe the stress field at the crack tip. The word “small” is technically undefined but a general guideline is shown in the following relationship:

$$\left(\frac{K_c}{\sigma_Y}\right)^2 \ll a \quad (1.1)$$

where, σ_Y is the yield strength of the material and a is the crack length. If this equation is satisfied then small scale yielding is assumed valid.

Once the stress intensity factor has exceeded the value of crack initiation toughness then subsequent crack growth is governed by a separate material property called the crack growth toughness, $K_c(\dot{K}, T, \dot{a})$. The crack growth toughness is postulated as a function of temperature, loading rate and crack speed, $\dot{a}$, which is the time derivative of the crack tip displacement. A third material parameter governs the arrest of a propagating crack. This crack arrest toughness is the smallest values of the dynamic stress intensity factor for which a moving crack cannot be maintained.

Of the three toughness parameters, the most interesting to engineers is the dynamic crack initiation toughness also sometimes referred to in literature simply as the dynamic fracture toughness. This is most important to engineers because ordinarily we only analyze the structural integrity of designs up to the onset of crack propagation. Once a crack has begun to propagate we usually consider the design failed. This is not always true, of course; for example, aircraft engineers have great interest in crack propagation as well as arrest.

In this dissertation, Chapter 2 will investigate the experimental work that has been

done to date in attempts to find different engineering materials' dynamic crack initiation toughness. Chapter 3 will present a novel experimental investigation of our own, followed by Chapter 4 and Chapter 5 which present peridynamic modeling of crack initiation.

1.2 Peridynamics

The peridynamic model [56, 57, 61] is a continuum reformulation of the classical partial differential equation of motion (conservation of momentum). It has been most notably used to model the deformation of bodies in which discontinuities (e.g., cracks) occur spontaneously. The basic equations are applicable even when singularities appear in the deformation field. These discontinuous deformations would lead to an inability to evaluate spatial derivatives in the classical formulation and special techniques would be required to analyze the problem. Recalling from classical continuum theory the conservation of momentum equation shown in Equation 1.2¹

$$\rho \ddot{\mathbf{u}}[\mathbf{x}, t] = \nabla \cdot \boldsymbol{\sigma}[\mathbf{x}, t] + \mathbf{b}[\mathbf{x}, t] \quad (1.2)$$

where, ρ , $\mathbf{u}$, $\mathbf{b}$ are statistically defined quantities representing continuum notions of mass density, vector valued displacement, and body force density, respectively. $\boldsymbol{\sigma}$ is a second order tensor which satisfies the equation, typically called the first Piola-Kirchhoff stress tensor. The independent variables $\mathbf{x}$ and t are defined as a position vector in the reference configuration and time, respectively.

In the peridynamic model, the second term on the right hand side of Equation 1.2, called the divergence of the stress tensor, is replaced with an integral functional. The functional relates pairwise forces or “bonds” between material particles in a continuum and is valid over any body without restriction on displacements (e.g., continuity, differentiability). The peridynamic equation of motion is given in Equation 1.3

$$\rho \ddot{\mathbf{u}}[\mathbf{x}, t] = \int_{\mathcal{H}} \mathbf{f}(\mathbf{u}[\mathbf{x}', t] - \mathbf{u}[\mathbf{x}, t], \mathbf{x}' - \mathbf{x}) dV_{\mathbf{x}'} + \mathbf{b}[\mathbf{x}, t] \quad (1.3)$$

where $\mathbf{x}'$ is the position vector of some neighboring material location with respect to $\mathbf{x}$ and $dV_{\mathbf{x}'}$ is the differential volume of $\mathbf{x}'$. $\mathcal{H}$ describes the family of continuum points $\mathbf{x}'$ with respect to $\mathbf{x}$. $\mathcal{H}$ is typically defined by a sphere of radius δ with center at $\mathbf{x}$. Figure 1.3a shows an illustration of a peridynamic continuum body, $\mathcal{B}$. It has been shown that if the analyst is only interested in the bulk response of the material then the choice of δ is essentially arbitrary [56]. However, if length scale is important, δ can be chosen appropriately, for example, to account for van der Waals forces in molecular dynamics modeling. It has also been proven [61] that Equation 1.3 reduces to the classical continuum partial differential equation in the limit as $\delta \rightarrow 0$, assuming a certain smoothness of the displacement field as required for the existence of partial derivatives.

¹Notation convention: Throughout this dissertation tensor quantities will be denoted by boldface type. First order tensors may be referred to in the text as vectors. States are denoted by uppercase bold letters with an underscore.

Figure 1.3: Schematic of peridynamic representations.

Equation 1.3 was the original formulation of the peridynamic theory, which carried a few significant shortcomings; mainly, it is an oversimplification to assume that any pair of particles interacts with each other only through a central force potential that is independent of all other local conditions. Therefore, for an isotropic, linear material there will always be an effective Poisson’s ratio of $1/4$, similar to Navier’s original elasticity theory. Another drawback to this particular model is the requirement to completely recast the constitutive behavior of a material in terms of a pairwise force function when, traditionally, material behavior has been formulated in terms of a stress tensor. Finally, although plasticity can be included in the bond-based theory by permitting permanent deformation of individual bonds, this results in permanent deformation of a material undergoing volumetric strain (without shear). Experimental observations of the behavior of metals have suggested that only shear deformations can involve plastic response.

With the need to address these issues, Silling et al. [59] reformulated the peridynamic theory to be more general. The resulting “state-based” peridynamic equation of motion² is given in Equation 1.4

$$\rho \ddot{\mathbf{u}}[\mathbf{x}, t] = \int_{\mathcal{H}} \{ \underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}', t] \langle \mathbf{x} - \mathbf{x}' \rangle \} dV_{\mathbf{x}'} + \mathbf{b}[\mathbf{x}, t] \quad (1.4)$$

where all the definitions for Equation 1.3 hold, and $\underline{\mathbf{T}}$ is defined as the peridynamic force-vector state. The concept of vector states is similar to that of a second order tensor in that they both map vectors into vectors, but vector states do not have to be linear or continuous functions. The angle brackets, $\langle \rangle$, in Equation 1.4 indicate the vector on which the state operates. $\underline{\mathbf{T}}$ maps a deformation-vector state into a force-vector state for each material point within $\mathcal{H}$. This generalization essentially allows for neighboring bonds to interact with each

²The formal derivation of this equation appears in Appendix F.

other and eliminates all of the shortcomings described above. Using this methodology there is a straightforward manner in which the analyst can take classical constitutive models (e.g., Hooke's Law) and convert them into force-vector state descriptions [59]. Equation 1.4 has also been shown to reduce to Equation 1.2 in the limit as $\delta \rightarrow 0$, again assuming a certain smoothness of the displacement field [60].

In order to solve general problems in solid mechanics Equation 1.4 is discretized and the integral is replaced with a finite sum. The resulting formula is shown in Equation 1.5

$$\rho \ddot{\mathbf{u}}[\mathbf{x}_i, t] = \sum_{j=1}^k \{ \mathbf{T}[\mathbf{x}_i, t] \langle \mathbf{x}_j - \mathbf{x}_i \rangle - \mathbf{T}[\mathbf{x}_j, t] \langle \mathbf{x}_i - \mathbf{x}_j \rangle \} V_j + \mathbf{b}[\mathbf{x}_i, t] \quad \forall i = 1, 2, \dots, \mathcal{N} \quad (1.5)$$

where $\mathbf{x}_i$ represents a discrete material particle, or node, and $\mathbf{x}_j$ represents a single node within the horizon, $\mathcal{H}$. k represents the total number of nodes within $\mathcal{H}$, and $\mathcal{N}$ represents the total number of nodes within the peridynamic body of interest. V_j is the volume of the $\mathbf{x}_j$ node. Figure 1.3b shows an illustration of a discretized peridynamic body $\mathcal{B}$. Figure 1.3b is shown with a structured grid of material points, however this is just for illustrative purposes as the grid could be completely random. This process is described in detail in Silling et al. [58], and results in a mesh free method of solving complex mechanics problems. An explicit time integration scheme is used to solve these equations for dynamic problems in the Sandia National Laboratories code, Emu. Emu discretizes a continuum body into nodes, each with a known volume in the reference configuration; this results in a meshfree method in the sense that there are no elements or geometric connectivities between the nodes. Emu has been used to solve many problems of interest for engineering communities who deal with projectile penetration and perforation, fragmentation, etc.

The common particle based numerical implementation of peridynamics often incorrectly draws comparisons with other particle methods [48, 13, 21], most notably the smooth particle hydrodynamics (SPH) method [45, 27]. These comparisons are generally a confusion of the numerical implementation with the underlying theory. Peridynamics is a complete continuum reformulation of the classical theory which provides significant advantages in the modeling of discontinuous displacements and problems involving length scale (because of the non-locality). The common comparison to SPH most likely results because of the appearance of an integral in the equations. In SPH, the material properties are smeared over a smoothing length, but the motion of the particles is still governed by partial differential equations; whereas, in peridynamics the motion of the particles is governed by intego-differential equations. Additionally the numerical implementation of peridynamics does not exhibit the tensile instability of SPH.

In this dissertation, we will use the state-based peridynamic method along with a novel failure model using dynamic crack initiation toughness measurements, implemented in Emu, to replicate the fracturing characteristics of a high-strength 4340 steel. Comparisons of the simulations are made to experiments.

2 Literature Review

2.1 Dynamic Fracture Experiments

In order to obtain an experimental measurement of a material’s dynamic crack initiation toughness a few essential elements are required. First, we obviously need a specimen with a sharp initial crack. This is typically done by growing a fatigue crack from the root of a sharp notch, sometimes called a precrack. ASTM E399 [29] outlines a typical procedure for generating the fatigue crack to ensure the “sharpness” of the crack tip. The next requirement is a method of generating a well controlled stress wave loading scheme. The final requirement is a way of instrumenting the specimen to gather information to reduce the dynamic stress intensity factor and also the time at which fracture occurs. The subsequent sections review a selection of the techniques in which other investigators have fulfilled these last two requirements.

2.1.1 Stress Wave Loading Techniques

Many experimental techniques have been used to generate loading at rates from essentially zero to around $10^8 \text{ MPa}\sqrt{\text{m}}/\text{s}$. The near zero loading rate schemes are typically called quasi-static tests and most commonly utilize precracked beams in bending or tension tests. These are generally carried out on a standard test apparatus (e.g., MTS[®] Machine) that has closed-loop feedback control to ensure the loading rate is constant. Static equations are then used to reduced the data to find the fracture toughness of the material.

Since there are not ASTM standards that govern the measurement of dynamic crack initiation toughness, experimentalists have tried many different techniques to generate the dynamic loading. The techniques include drop-weight tower, projectile impact testing, Kolsky bar methods, explosive loading, and electromagnetic loading schemes. In most of these techniques it can be difficult to accurately control the stress wave loading pulse. The techniques that offer the most control of the shape and duration of the loading pulse are the Kolsky bar methods and the electromagnetic scheme. Table 2.1 provides a summary of the mode I loading rates that each of these methods are capable of achieving and the approximate time to fracture, t_f , for each method. The Kolsky bar methods are included within

Table 2.1: Stress wave loading schemes and respective loading rates.

	Quasi-static Loading Machines (MTS)	Drop-Weight Towers	Projectile Impact	Explosives	Electromagnetic Loading Schemes
$\dot{K}_I$ (MPa $\sqrt{\text{m/s}}$)	1	10^4	$10^4 - 10^6$	10^8	10^5
t_f (μs)	$> 10^6$	100	1 – 100	1 – 20	10 – 100

projectile impact category. The remainder of this section will take a closer look at the most valid ways of conducting dynamic crack initiation testing.

Electromagnetic Loading

The electromagnetic scheme introduced by Ravi-Chandar et al. [49, 50] is a novel method in which current carrying conductor plates are attached to opposite sides of an existing crack on a specimen. A similar charge is applied to each plate through a capacitor bank which causes the plates to repel and the crack to propagate. The authors indicate that the time history of the loading pulse can be shaped through the choice of capacitors and inductors in the circuitry. One of the biggest advantages to this method is that the experimental configuration replicates very closely the loading model of a pressurized semi-infinite crack in an unbounded medium for which a closed form solution for the dynamic stress intensity factor can be obtained [17, 18]. While this method seems to provide an excellent way for generating well controlled repeatable stress waves, it has only been demonstrated on certain low strength materials such as polymers. Whether or not this method can feasibly be extended to high strength materials like steel is unproven. It may be impracticable and unnecessarily dangerous to engineer a capacitor bank that can deliver the necessary repulsive force to cause a crack to propagate in a high strength steel.

Kolsky Bar Loading

Kolsky bar, also known as split-Hopkinson bar, experimental methods [28, 38, 39, 22, 10, 19, 11, 20] are well known techniques for performing high-rate material testing, usually to produce stress-strain relationships at strains rates from $10^2/\text{s}$ to $10^4/\text{s}$. A minimal Kolsky apparatus consists of an incident, transmission, and striker bar, all cylindrical in geometry, and typically with length to diameter ratios of greater than 20 to ensure one-dimensional wave propagation. Traditionally, the striker bar is propelled into the end of the incident bar imparting a stress (or strain) wave which propagates to a cylindrical sample that is sandwiched between the incident and transmission bars. The compressive wave created by striking the incident bar with the striker is called the incident wave, the wave that is reflected back in tension through the incident bar is called the reflected wave, and the compressive wave that travels through the sample into the transmission bar is called the transmitted

wave. Figure 2.1 shows a schematic of a Kolsky bar. Strain gages are typically placed on the surface of the incident and transmission bars and the measured strains can be related to material properties in the sample. The material properties of interest in a traditional Kolsky bar test are typically curves showing stress as a function of strain at known strain rates. The following equations will derive how these measures are arrived at in a traditional test. First, we know that engineering strain, ε , is typically defined as follows:

$$\varepsilon(t) = \frac{L_f(t) - L}{L} \quad (2.1)$$

where, $L_f(t)$ and L are final and initial lengths, respectively. If we refer to Figure 2.1 and define $x_1(t)$ and $x_2(t)$ as the positions of locations 1 and 2 then at any time t , $L_f(t) = x_2(t) - x_1(t)$. Substituting this relationship into Equation 2.1 we have:

$$\varepsilon(t) = \frac{x_2(t) - x_1(t) - L}{L} = \frac{x_2(t) - x_1(t)}{L} - 1 \quad (2.2)$$

By taking the first derivative with respect to time of Equation 2.2 we can define the engineering strain rate as follows:

$$\dot{\varepsilon}(t) = \frac{\dot{x}_2(t) - \dot{x}_1(t)}{L} = \frac{v_2(t) - v_1(t)}{L} \quad (2.3)$$

where, v_1 and v_2 are the velocities of locations 1 and 2 in Figure 2.1. We wish to relate these velocities to the measured values of strain recorded in the strain gages on each bar. From one-dimensional wave theory [39, 22, 43] we know the following relationship for the particle velocity, U_p , in a one-dimensional rod:

$$U_p = c\varepsilon \quad (2.4)$$

where, c is the wave speed and ε is the strain in the bar. Therefore, at interfaces 1 and 2 we have the following:

$$1 \rightarrow v_1(t) = c_0(\varepsilon_I(t) - \varepsilon_R(t)) \quad (2.5)$$

$$2 \rightarrow v_2(t) = c_0\varepsilon_T(t) \quad (2.6)$$

Figure 2.1: Schematic of Kolsky bar.

where, c_0 is the wave speed of the incident and transmission bars, ε_I refers to the measured strain from the incident strain wave, ε_R refers to the measured strain from the reflected strain wave, and ε_T refers to the transmitted strain wave. The reason the $(\varepsilon_I - \varepsilon_R)$ term appears in Equation 2.5 is because there is an impedance mismatch at the interface of the incident bar and the sample which causes some of the strain wave to propagate into the sample and some to be reflected back. We can now substitute Equation 2.5 and Equation 2.6 into Equation 2.3 and simplify to get the following relationship for engineering strain rate:

$$\dot{\varepsilon}(t) = \frac{c_0}{L} (\varepsilon_I(t) - \varepsilon_R(t) - \varepsilon_T(t)) \quad (2.7)$$

Equation 2.7 can now be integrated over time to find the engineering strain in the sample as shown in Equation 2.8.

$$\varepsilon(t) = \frac{c_0}{L} \int_0^t (\varepsilon_I(t) - \varepsilon_R(t) - \varepsilon_T(t)) dt \quad (2.8)$$

In order to find the stress we will assume equilibrium over the entire sample, therefore the stress can be found in terms of the force on each end of the sample as follows:

$$\sigma(t) = \frac{P_1(t) + P_2(t)}{2A} \quad (2.9)$$

where, σ is the stress in the sample, P_1 and P_2 are the force applied to the sample at the interface, and A is the cross sectional area of the sample. The forces can be evaluated from the incident and transmission bar strains at the interfaces as follows:

$$1 \rightarrow P_1(t) = A_0 E_0 (\varepsilon_I + \varepsilon_R) \quad (2.10)$$

$$2 \rightarrow P_2(t) = A_0 E_0 \varepsilon_T \quad (2.11)$$

where, A_0 is the cross-sectional area of the bars and E_0 is the elastic modulus of the bars. Substituting Equation 2.10 and Equation 2.11 into Equation 2.9 results in Equation 2.12.

$$\sigma(t) = \frac{A_0 E_0}{2A} (\varepsilon_I(t) + \varepsilon_R(t) + \varepsilon_T(t)) \quad (2.12)$$

But, for equilibrium, $P_1 = P_2$ and therefore $\varepsilon_I + \varepsilon_R = \varepsilon_T$. If we substitute this back into Equation 2.7, Equation 2.8, and Equation 2.12 we can get the final equations used to reduce stress-strain relationships from Kolsky bar experiments. These equations are shown below:

$$\sigma(t) = E_0 \frac{A_0}{A} \varepsilon_T(t) \quad (2.13)$$

$$\dot{\varepsilon}(t) = -\frac{2c_0}{L} \varepsilon_R(t) \quad (2.14)$$

$$\varepsilon(t) = -\frac{2c_0}{L} \int_0^t \varepsilon_R(t) dt \quad (2.15)$$

These are the standard equations found in many texts and typically presented in literature without derivation.

In the last thirty years the Kolsky bar testing methods have been extended to dynamic fracture testing. Researchers have used one, three, and four point bend specimens in a multitude of configurations. Many have used novel specimen designs in tension, compression and wedging tests. The remainder of this section will be dedicated to reviewing a selection of relevant research using the Kolsky bar.

One of the earliest adaptations of the Kolsky bar technique for fracture testing was developed by Costin et al. [12]. A 25.4 mm diameter bar with a fatigued radial notch was loaded with a tensile stress pulse originating from an explosive detonation. Using the standard equations for Kolsky bar data reduction the average stress at the crack tip was calculated. Crack tip opening displacement was also measured with a moiré optical method thus yielding a load displacement record of the fracture event. The authors used this method to determine the rate dependence of the dynamic crack initiation toughness at loading rates on the order of $10^6 \text{ MPa}\sqrt{\text{m}}/\text{s}$ for SAE 4340 steel and 1020 cold-rolled steel. One issue noticed in this paper related to the reporting of loading rates as constant values, because of the explosive loading scheme the load-time history is parabolic in nature at the onset of the load. For a near constant loading rate the load-time history should be near linear. Overall this work produced reasonable data and showed the Kolsky bar as a viable resource for dynamic fracture testing. The use of explosives and the advent of newer loading methods would deter most researchers from replicating these procedures exactly.

Rittel et al. [52] used a Kolsky bar setup with a novel specimen design called the *compact compression specimen* which was placed in between the incident and transmission bars of the Kolsky apparatus. The compact compression specimen allowed for the crack to open when impacted with a compressive incident wave. Specimens were made of 1035 steel with a precrack cut with a diamond wire. The root radius of the crack was reported as 0.17 mm. A fracture gage (timing wire) was painted using conductive silver paint very close to the crack tip and sequenced with the incident stress pulse in order to get the time-to-fracture. The authors realized that although the compact compression specimen allowed for a simple test procedure, it induces asymmetries in the the loading process, therefore the specimen was not in dynamic equilibrium and mixed mode I and II opening also occurred during fracture. Since a quasi-static analysis was not valid, a procedure for finding the dynamic crack initiation toughness was used. Analysis taken from [7] shows that for a non-propagating side crack of length, a , in an semi-infinite two dimensional body, S , for a linear-elastic material the authors define the H -integral as shown in Equation 2.16.

$$H := \frac{1}{2} \int_S \mathbf{T}[\mathbf{u}] * \frac{\partial \mathbf{v}}{\partial a} dS = \frac{1 - \nu^2}{E} K_I^{\mathbf{u}} * K_I^{\mathbf{v}} \quad (2.16)$$

where $\mathbf{u}$ is the displacement field in S to which the dynamic load $\mathbf{T}[\mathbf{u}]$ is applied. $\mathbf{v}$ is a reference field and $*$ is the time convolution product¹. $K_I^{\mathbf{u}}$ and $K_I^{\mathbf{v}}$ are defined as the dynamic stress intensity factors associated with $\mathbf{u}$ and $\mathbf{v}$ respectively. $\mathbf{u}$ and $\mathbf{T}[\mathbf{u}]$ are determined experimentally for each test performed. $\mathbf{v}$ and $K_I^{\mathbf{v}}$ are determined numerically through a finite element model (FEM) simulation that only needs to be done once. Finally, an algorithm is used to solve the linear convolution equation for $K_I^{\mathbf{u}}$, at the time of fracture

¹ $f(t) * g(t) = \int_{-\infty}^{\infty} f(\tau) \cdot g(t - \tau) d\tau$

$K_I^u = K_{Ic}$. The authors report a dynamic crack initiation toughness for the 1035 steel of $180 \text{ MPa}\sqrt{\text{m}}$, but recognize this number to most likely be incorrect because of the relatively blunt crack tip. The most apparent drawback of this method is the need to calculate $\mathbf{v}$ and K_{Ic}^y via FEM. Using this procedure the accuracy of K_{Ic} is based on the accuracy of the FEM results. Most likely in order to obtain accurate FEM calculations one would need to have an extremely high mesh density in the crack tip region which could prove to be too computationally expensive to be practical. The authors also describe “filtering” out of the mode II stress intensity factor, but do not go into detail about the procedure used.

Klepaczko [37] provides a detailed review of many experimental procedures used in dynamic crack initiation testing including a method of his own design using the *wedge loaded compact tension* (WLCT) specimen. This method attaches a compressive wedge to the incident bar and places the WLCT specimen between the wedge and the transmission bar. Estimates were made for the transverse inertia of the WLCT specimen during loading as well as frictional effects. It was concluded through this analysis that as long as the fracture time was longer than the initial rise time of the incident pulse the inertia and frictional effects essentially canceled each other out. One issue to note was that the frictional force was modeled with a simple Coulomb friction law which may not be adequate in this dynamic loading regime and could introduce errors into the calculation of K_{Ic} . It appears that Klepaczko calculates the time-to-fracture simply by inspecting the reflected strain data recorded on the oscilloscope looking for what he calls “pop-in” points. The author reports results from WLCT tests on aluminum alloys conducted over seven decades of loading rate. The results show a drop in K_{Ic} at $\dot{K}_I \approx 10^2 \text{ MPa}\sqrt{\text{m}}/\text{s}$.

A different set of dynamic crack initiation toughness experiments on 2024-T3 aluminum was conducted by Owen et al. [46]. The authors used thin aluminum sheets in both a MTS[®] load frame for $\dot{K}_I < 10^2 \text{ MPa}\sqrt{\text{m}}/\text{s}$ and a Kolsky tension bar test configuration for $\dot{K}_I > 10^5 \text{ MPa}\sqrt{\text{m}}/\text{s}$. The specimens were cut with wire electrical discharge machining (EDM) before being fatigued in a MTS[®] machine to produce a sharp crack. The values of K_{Ic} were found via the standard quasi-static means for the MTS[®] machine experiments. For the Kolsky tension bar tests four-angle steel tabs were attached to each side and at both ends of the specimen. The specimen was then placed in mating fixtures which were threaded into the end of each bar. The authors report that the specimen did not slip with respect to the steel tabs during the test. The tensile stress in the specimen is calculated via standard Kolsky bar techniques using the transmitted strain signal and related to the dynamic stress intensity factor by Equation 2.17 taken from [1]:

$$K_I(t) = \frac{\sigma(t)W}{\sqrt{W}} \frac{\sqrt{2 \tan\left(\frac{\pi a}{2W}\right)}}{\cos\left(\frac{\pi a}{2W}\right)} \times \left[0.752 + 2.02 \left(\frac{a}{W}\right) + 0.37 \left(1 - \sin\left(\frac{\pi a}{2W}\right)\right)^3 \right] \quad (2.17)$$

where W is the width of the sample, and $\sigma(t)$ is the applied stress. $\dot{K}_I$ was calculated using a least squares fit to the $K_I(t)$ curve and the dynamic crack initiation toughness, K_{Ic} , was taken as the point where a line having a slope of $0.95\dot{K}_I$ intersected the $K_I(t)$ curve. This

is the same procedure used for finding the fracture toughness in quasi-static tests [29].

Equation 2.17 was derived without taking inertia effects into consideration, therefore to simply replace the quasi-static stress, σ , with a time dependent load, $\sigma(t)$, is only valid if the sample is shown to be in dynamic stress equilibrium. Owen et al. used an independent local measurement on one test to help validate the use of the time varying boundary load results. They used an optical method to measure the local crack tip opening displacement (CTOD). The J -Integral was evaluated using a relationship given by Shih [54]. When the CTOD is measured at the intersection of two lines at 45° with respect to the crack line the relationship is shown in Equation 2.18,

$$CTOD = d_n(\varepsilon_0, \alpha, n) \frac{J}{\sigma_0} \quad (2.18)$$

where, the parameter d_n is a function of the reference strain, ε_0 , constitutive parameters, α and n , and stress state, σ_0 . Equation 2.18 can be solved for J and then the J -Integral can be related to the fracture toughness by the well known equation for plane stress shown in Equation 2.19.

$$J = \frac{K_{Ic}^2}{E} \quad (2.19)$$

A limitation of this technique is that in order to extend it to the dynamic regime you must know the correct high-rate constitutive parameters contained in d_n to be able to calculate J accurately. The data is then reported for K_{Ic} as a function of $\dot{K}_I$. The local CTOD values for K_{Ic} are overlaid with associated boundary load K_{Ic} measurements. Owen et al. make the statement that for times greater than $20 \mu s$ there is good comparison between the two calculated values. One key flaw in this approach is with the method of calculating the dynamic crack initiation toughness. The investigators in this paper use a 5% offset value from a linear line drawn through the rise of the loading pulse. This is how K_{Ic} is calculated in quasi-static testing per ASTM E399. In dynamic testing an accurate time-to-fracture should be calculated experimentally because inertia in either the sample or the loading fixture can cause the recorded load to continue rising after crack initiation. Additionally, the constant approximation for loading in this case was not accurate because the $K_I(t)$ curve oscillated before the fracture time. This state of constant loading is assumed when they generate a plot of K_{Ic} as a function of $\dot{K}_I$. The highest loading rates were on the order of $10^6 \text{ MPa}\sqrt{\text{m/s}}$; at these rates there is a drastic increase in dynamic crack initiation toughness. This is in stark contrast to the observations of Klepaczko whose work showed a decrease in K_{Ic} at the highest rates. The two experimental results are compared in Figure 2.2 Granted Klepaczko's experiments were close to plane strain loading whereas Owen et al. was close to plane stress, and the aluminum used in each respective test are not the exact same alloy. One would expect to get different values of K_{Ic} in these two experiments, but the opposing trends in rate dependence are somewhat alarming.

Yokoyama et al. [69, 68] used a modified Kolsky bar assembly to conduct three point bend dynamic crack initiation experiments. Two transmission bars were used as the supports for a precracked beam and the incident bar was used to apply the dynamic load. The time-to-fracture is found by mounting a semiconductor strain gage on the specimen and using the

Figure 2.2: Comparison of experimental results from Klepaczko and Owen.

peak strain as the time when the crack initiates. The boundary load histories are then input into a finite element model and combined with the time-to-fracture information to extract the dynamic crack initiation toughness. Like other methods that use FEM to extract $K_I(t)$, they are only valid if you have an accurate FEM model.

Popelar et al. [47] used a very well instrumented modification of a Hopkinson bar in three point bend tests of a precracked beam. The dynamic load was applied through the incident bar which records the incident pulse. The samples were instrumented with strain gages to monitor the sample contact with the support pins to ensure the beam was not set into resonance and “jump” off the supports. An eddy current sensor was used to monitor CTOD. There is also a crack ladder gage to measure time-to-fracture and give a discrete measurement of crack growth speed. The authors use what they call a quasi-dynamic model to extract the dynamic stress intensity factor from the CTOD data. Their model comes from a solution for the CTOD produced by Tada et al. [65] for a *propagating* crack. For brevity these equations are omitted here, however in calculating the dynamic stress intensity factor, and in turn its critical value, K_{Ic} , from these equations for a propagating crack they are failing to consider the dynamic crack initiation toughness and dynamic crack propagation toughness as independent material properties as suggested by other researchers [49, 18].

Jiang et al. [32] used a Kolsky pressure bar in modified Charpy impact tests to find the dynamic crack initiation toughness of steel specimens. The specimen is supported by an anvil and loaded with the incident bar from the Kolsky apparatus. The authors use a model based on a simple spring-mass system to provide an equation for the dynamic motion of

the precracked beam. They model the beam as three point bending and use a linear elastic mechanics approach to solve for the stiffness of the beam and in turn derive an expression for the dynamic stress intensity factor. The final expression they used is shown in Equation 2.20.

$$K_I(t) = \frac{3S\sqrt{a}}{2BW^2} Y\left(\frac{a}{W}\right) \omega_1 \int_0^t P(\tau) \sin \omega_1 (t - \tau) d\tau \quad (2.20)$$

Where, a is the crack length, W is the width of the specimen, B is the thickness of the specimen, S is the distance between the supports, and $Y\left(\frac{a}{W}\right)$ is a compliance function taken from Srawley [63]. $P(\tau)$ is the recorded boundary load from the incident bar strain gage and ω_1 is the natural frequency of vibration which is a function of the calculated stiffness $K(a)$. Equation 2.20 is then integrated and combined with the measured time-to-fracture from the experiment to find K_{Ic} . The details of this procedure are laid out in [32]. Rokach, in his rebuttal to Jiang et al.'s paper [53] noticed an error in these approximations. The average time-to-fracture in the reported experiments was less than $13\mu\text{s}$ which is faster than the time it takes a dilatational wave to travel from the impact boundary to the supports and return to the crack tip. Therefore the crack does not even see the effect of the supports, this is generally referred to as one point bending. Due to the conditions of one point bending, the analysis Jiang et al. used to determine the dynamic stress intensity factor is not valid because it was derived based on three point bending.

More recently, Weerasooriya et al. [67] used a four point bend technique to determine the dynamic crack initiation toughness in ceramics. They used a modified Kolsky setup with the specimen loaded in four point bending between the incident and transmission bars. They used a pulse shaping technique [19, 20] to carefully control the loading pulse to ensure not only constant loading rate, but dynamic equilibrium of the sample as well. Quartz force transducers were imbedded in the ends of the incident and transmission bars to measure the sample in equilibrium. Because the sample was shown to be in dynamic stress equilibrium, quasi-static analysis was used to find the dynamic crack initiation toughness. These experiments were performed at loading rates of $4 \times 10^4 \text{ MPa}\sqrt{\text{m}}/\text{s}$ and $1.5 \times 10^5 \text{ MPa}\sqrt{\text{m}}/\text{s}$, and showed dynamic crack initiation toughness measurements of $5.5 \text{ MPa}\sqrt{\text{m}}$ and $9.5 \text{ MPa}\sqrt{\text{m}}$, respectively.

In one of the most recent works to date, Jiang et al. [34] have devised a new experimental technique using a what they call two-bar/three point bending. This is a much improved technique over the incident bar Charpy scheme by the same authors reviewed earlier. Similar to work by Weerasooriya et al. these investigators use a traditional two bar Kolsky apparatus experimental setup with a three point bending mechanism attached to the incident and transmission bars. Figure 2.3 shows a schematic of the gage section between the incident and transmission that facilitates the three point bending. They use pulse shaping techniques to control the incidence pulse and investigate the loss of contact issue between the impact pins and the specimen. They use a clever voltage scheme to monitor the contact at the pins and show that the loss of contact occurs well after the crack initiates in the sample. The authors do not actually report any calculated values for dynamic stress intensity factor, but show this techniques applicability for use in dynamic crack initiation testing of both steel and aluminum samples. Dynamic stress equilibrium is verified with the 1-wave 2-wave

Figure 2.3: Schematic of Jiang three point bend setup.

technique. The only possible issue noted with this work has to do with the possibility of not having pure mode I opening. The authors provide a sample of high-speed photographs as validation of their voltage contact measurement and in these photographs the crack does not appear to propagate straight across the sample. This “turning” action exhibited by the crack propagation indicates that mixed mode opening is occurring. However this could possibly be due to slight misalignment and easily corrected.

In what is most likely the most recent published work, Jiang et al. [33] modified the experimental technique described in the last paragraph to employ four point bending instead of three. All other aspects of the setup were essentially the same. The four point bending should eliminate any misalignment issues and ensure pure mode I opening during crack initiation. However, they did not report any actual experimental values of dynamic crack initiation toughness, they only evaluated the experimental technique.

In this research, a similar method to those described by Jiang et al. and Weerasooriya et al., is used to record the dynamic crack initiation toughness measurements of a 4340 steel at two different nominal loading rates.

2.2 Peridynamics

The peridynamic theory of solid mechanics is a relatively new development in continuum modeling. There have been only 15-20 papers written on the subject, several of which are cited elsewhere in this dissertation. The following few paragraphs review some of the key articles written on the subject as well as other techniques in computational modeling of material failure.

The original paper on peridynamics was published by Silling in the year 2000 [56]. This paper introduced what is now called “bond” based peridynamics, introduced several prototype material models, and compared several mathematical notions to their analogs in classical mechanics (partial differential equation) theory. The paper demonstrated the straightforward emergence and modeling of discontinuities (e.g., cracks) without the need for special, sometimes artificial, mathematical models to handle them.

A paper that examined some interesting behavior of the peridynamic theory was published by Silling et al. [61]. In this paper the authors analyzed the deformation fields in a one dimensional infinite peridynamic bar. Some interesting phenomenon was shown that is not realized in the classical theory. For instance, the equilibrium solution of the bar for the displacement field has the same smoothness as the body force field being applied to the bar. In the classical theory of elasticity the displacement field would be two orders smoother (i.e., continuously differentiable) than the body force field.

The first publication on the numerical implementation of peridynamics was authored by Silling and Askari [58]. In this paper, the authors discretize and numerically implement the peridynamic continuum model, give an example of a prototype microelastic constitutive model, and present example problems where discontinuities arise naturally as part of the deformation. This paper also presented a derivation of a failure criterion based on energy release rate that arrives at a critical bond stretch at which a bond will fail irreversibly once exceeded.

In order to address the shortcomings described in Chapter 1 of the “bond” based peridynamic model, a generalization was done and published by Silling et al. [59]. The outcome of this paper is what is now referred to as “state” based peridynamics. This generalization introduced the notion of peridynamic vector-states which allows for more complex material models while retaining the ability to model complex and even discontinuous deformations. The theory presented in this paper was later shown by Silling and Lehoucq [60] to converge to the classical theory in the sense of a limit as the non-local horizon tends to zero. This convergence is based on several assumptions including a homogenous, smooth deformation field.

Because the numerical implementation of peridynamics is a Lagrangian formulation that represents each discrete material point as a particle, it often draws comparisons to other so called particle methods from the classical theory. These include smooth-particle hydrodynamics (SPH) [45, 27], element-free Galerkin (EFG) methods [4, 41, 5, 6], and reproducing-kernel particle method (RKPM) [40, 9]. It is important to remember that these other numerical techniques arise from the weak form of the classical partial differential equations and require special mathematical techniques to account for the spontaneous evolution of discontinuities. In the use of the finite element method for crack propagation, artificial numerical “trickery” is sometimes resorted to in order to handle discontinuities. These include element death (deletion), element-to-particle conversion [36], cohesive zone elements [16], and extended finite elements (XFEM) [44, 64]. While all of the aforementioned methods have been demonstrated to varying degrees of accuracy with respect to their application on problems of fracture, all of them require the application of an external model, not inherent to the fundamental equations, to describe these material failures.

To illustrate the versatility of the peridynamic theory, please allow the use of the following analogy:² Assume there are a set of equations which accurately describe the atmospheric weather on most days, including sunny days, raining days, snow days, etc., but are inca-

²Credit is respectfully give to Dr. Stewart A. Silling for the originality of this analogy.

pable of describing truly adverse weather such as tornadoes, hurricanes, and blizzards. Now assume that these equations are implemented into a numerical code using the finite element method and the finite element code could replicate the physics of the underlying equations by predicting the weather on most days, but in order to model adverse weather, the analyst had to employ the use of “special” elements, e.g., tornado elements. This is equivalent to the idea of using cohesive zone elements (and other special numerical techniques) to model fracture. Even though they perform adequately, they represent a significant departure from the underlying theory. The peridynamic theory circumvents the need for external equations to model the adverse events, such as fracture. The peridynamic theory of solid mechanics captures all of this while showing significant tiebacks to the classical theory and retaining the ability to model more conventional continuous deformations.

3 Experimental Procedure

3.1 Introduction

This chapter introduces the technique used to experimentally determine the dynamic crack initiation toughness of a 4340 steel. While the technique is not entirely novel [33, 34, 67], this is the first time it has been presented in this exact configuration. At the outset of this research one goal was to achieve a standard technique for establishing the crack initiation toughness of metallic materials at dynamic loading rates in a similar fashion to the ASTM standard E399 for finding fracture toughness in metals at quasi-static loading rates. The research presented herein provides an approach that the author believes is an improvement on other techniques found in literature, it can be used to provide accurate results at known dynamic loading rates, but still has a few shortcomings to be improved upon in future iterations. These shortcomings do not involve accuracy of the results only the ease in which the experiments can be conducted and the data reduced, all of which will be mentioned along with suggestions for further improvement. This chapter includes detailed descriptions of the processes of sample preparation, fatigue precracking, and fracture time detection which are often overlooked or presented as trivial issues in the dynamic fracture literature. A detailed description of the modified Kolsky bar and data reduction techniques is also provided in this chapter.

3.2 Sample Preparation

ASTM E399 provides guidelines for the sample preparation of compact tension specimens, notched tensile specimens, and three point bend beam specimens for the purpose of experimentally detecting quasi-static fracture toughness values. For dynamic crack initiation toughness testing, we have established in Section 2.1.1 that the most common method and easiest way to deliver controlled dynamic loading is the Kolsky apparatus. For this reason and others to be elaborated on subsequently, the Kolsky bar was the method we chose to apply the dynamic loading in the dynamic crack initiation tests. In an attempt to follow the spirit of ASTM E399, the bend beam sample was chosen as the sample configuration. However the experiments we conducted were a four point bend configuration as opposed to

Figure 3.1: Four point bend beam.

a three point bend. This was done because alignment is not as critical in a four point bend test. In a three point bend test even the smallest misalignment of the striking tup with the crack can cause mixed mode opening of the crack tip which is undesirable when attempting to capture K_{Ic} . When doing quasi-static tests, alignment is not very hard to achieve because the tests are generally done in a standard test apparatus (e.g., MTS[®]) where the sample, supports, and striking tup all sit in a vertical orientation, respectively. In the Kolsky bar the striking tup is on the incident bar end and the sample is supported only by a small amount of friction between the tup and supports and arranged in a horizontal fashion. This arrangement lends itself to the possibility of slippage between the sample and supports. As long as the potential slippage is small and the crack tip remains between the two striking tups, the sample will experience pure bending and mode I opening will be ensured. This horizontal arrangement was also the reason why the compact tension specimen was not considered, since the size of the sample is much too large to be held in place only by the friction of the supports and tups. The notched tensile specimen could be considered for use in the Kolsky apparatus, but the additional and unnecessary complication of a tensile Kolsky bar was the reason that sample was not considered.

Figure 3.1 shows an illustration of a four point bend precracked beam with descriptive labels for relevant geometries. ASTM E399 states that the relationship between the sample thickness, B , and sample width, W , should be $B = W/2 \pm 0.010W$ and the length, L , should be a minimum of $4.2W$. The total length of the crack, a , which includes the total dimension of the starter notch and the fatigue generated precrack should be between $0.45 \leq a/W \leq 0.55$. The generation of the fatigue precrack is discussed in detail in Section 3.3. Based on the ASTM E399 guidelines the nominal sample dimensions used in the Kolsky bar tests are shown in Table 3.1. Machine drawings for the samples are included in Appendix C, and the

Table 3.1: Nominal sample dimensions.

W	B	L	a
15 mm	7.5 mm	63.5 mm	7.5 mm

actual measured dimensions of each sample used for testing is included in Appendix D.

Each sample was machined from 4340 plate stock that originally had rough dimensions of approximately $130\text{ mm} \times 80\text{ mm} \times 10\text{ mm}$. Before machining the plates were heat treated with the following procedure:

1. Annealing: Heat at 680°C for 8 hours, air cool
2. Strengthening: $845^\circ\text{C} \pm 10^\circ\text{C}$ for 1 hour at temperature, oil quench
3. Temper: $200^\circ\text{C} \pm 10^\circ\text{C}$ for 1 hour at temperature, air cool

After heat treatment the samples were machined using a wire EDM to the final dimensions. A starter notch was cut to a depth of 5 mm, the thinnest possible width (maximum of 2 mm), and perpendicular to the edge within 2° to facilitate fatigue cracking. The front and back faces were finally machine ground to a surface finish of $3.2\text{ }\mu\text{m}$. This process resulted in samples with Rockwell C50-C55 hardness.

The final step of sample preparation was to polish one side of the sample to a mirror finish and label each with a serial number. The mirror finish allowed for easy visibility of the fatigue crack under the microscope during the fatigue crack growth process.

3.3 Fatigue Cracking

ASTM standard E399 states that even the narrowest practical machined notch cannot simulate a natural crack well enough to provide a satisfactory measurement of K_{Ic} . Therefore, it is necessary to artificially create a sharp crack by initiating and growing a fatigue crack from the root of a narrow machined notch before attempting any K_{Ic} measurements. To ensure the crack is sufficiently “sharp”, ASTM E399 gives guidelines for so called K -calibration. ASTM E399 also gives guidelines for the appropriate crack length and approximate number of cycles it should take to grow the fatigue crack. A summary of these guidelines are given as follows:

- The maximum stress intensity factor, K_{max} , during any stage of fatigue crack growth shall not exceed 80% of the resulting K_{Ic} .¹
- For the terminal stage of fatigue cracking (the final 2.5% of the intended crack size, a), K_{max} shall not exceed 60% of the resulting K_{Ic} .
- The final crack length, a , should be between $0.45W$ and $0.55W$.

¹For the first test of a new material, K_{Ic} may be unknown; therefore, an estimation may have to be used, and if the resulting $K_{Ic} > 1.2K_{max}$, the fatigue process and experiment will have to be repeated with corrections in order for K_{Ic} to be assumed valid.

- The total number of cycles to generate the fatigue crack should be between 10^4 and 10^6 .

The load for the fatigue cracking procedure was generated using a four point bend fixture in an 4.5 kN MTS[®] servo-hydraulic test frame, Model 312.21. The K -calibration was done by running the load frame in force control mode, cycling the appropriate load. In order to calculate the appropriate load levels for sufficient K -calibration we must first solve for the load, P , from the stress intensity factor definition. For a four point bend beam in mode I loading, the stress intensity factor is calculated by Equation 3.1 [65]

$$K_I = \frac{6M}{BW^2} \sqrt{\pi a} \cdot \beta \left(\frac{a}{W} \right) \quad (3.1)$$

where, the definitions from the Section 3.2 hold, and M is the applied moment defined by:

$$M = pd \quad (3.2)$$

and the compliance function, β , is defined by:

$$\beta \left(\frac{a}{W} \right) = 1.22 - 1.40 \frac{a}{W} + 7.33 \left(\frac{a}{W} \right)^2 - 13.08 \left(\frac{a}{W} \right)^3 + 14.00 \left(\frac{a}{W} \right)^4 \quad (3.3)$$

In Equation 3.2, p refers to the force applied at each of the four support locations and d is the span between the four point bend supports. Defining the force at each of the supports in terms of the force measured by the MTS[®] test frame, P , we have,

$$p = \frac{P}{2} \quad (3.4)$$

Now substituting Equation 3.4 into Equation 3.2 and then that result into Equation 3.1 and solving for P we have the following relationship:

$$P = \frac{K_I BW^2}{3d \sqrt{\pi a} \cdot \beta \left(\frac{a}{W} \right)} \quad (3.5)$$

Following the guidelines listed earlier in this section, at no stage during fatigue crack growth did K_I in Equation 3.5 exceed $K_{max} = 0.8K_{Ic}$. The assumption was made that the dynamic crack initiation toughness was greater in magnitude than the quasi-static fracture toughness. For most heat treatments of 4340 steel the reported fracture toughness, K_{Ic} , is approximately $65 \text{ MPa}\sqrt{\text{m}}$. Rounding down to be conservative $K_{max} = 50 \text{ MPa}\sqrt{\text{m}}$ was used for the fatigue crack initiation. For the terminal growth of the fatigue crack, $K_{max} = 39 \text{ MPa}\sqrt{\text{m}}$ was used. In order to calculate the load, P , the crack length, a , corresponding to the expected final length of approximately 7.5 mm was used. This added additional conservatism to the calculation of P because initially the crack length was smaller than 7.5 mm; therefore, the actual value of K_I was initially lower and increased to the value of K_{max} as the crack was grown. Using the nominal sample dimensions described in Section 3.2 and $d = 17.33 \text{ mm}$, the initial and terminal values of P were calculated to be 9.34 kN and 7.12 kN, respectively.

In order to initiate the fatigue crack, the MTS[®] test frame was placed in force control mode and cycled between 0 and 9.34 kN at a rate of 50 Hz. A KEYENCE digital microscope with integrated imaging, Model VHX 100K, was used to monitor the fatigue crack initiation and growth. Figure 3.2 shows the four point bend fixture in the MTS[®] test frame with the sample in place and the microscope camera lense. Figure 3.3 shows a fatigue crack being monitored. The mirror surface finish on the sample allowed the fatigue crack to be clearly monitored during growth. The blue line to the left of the growing crack in Figure 3.3 represents a distance of nominally 2 mm. Once the fatigue crack initiated the force was lowered to cycle between 0 and 7.12 kN, once again at a rate of 50 Hz until the crack length was near the overall desired length of nominally 7.5 mm. The entire fatigue crack initiation and growth took approximately 15 minutes per sample, and resulted in approximately 45 000 cycles. The fatigue crack initiation and growth was a very repeatable process. The fatigue crack growth rate was easily controlled by gradually lowering the force as the crack neared the desired length; which, resulted in a very “sharp” crack tip of nearly equal length for all samples.

3.4 Apparatus

To apply the dynamic loading for these experiments a modified Kolsky bar, also known as a split-Hopkinson pressure bar (SHPB), at Sandia National Laboratories was used. The Kolsky bar is an apparatus consisting of two long cylindrical bars, identified as the incident and transmission bars respectively, and a striker bar. It is typically used for the characterization (i.e., stress-strain data) of engineering materials at high strain rate. This is done by placing a small specimen, between the incident and transmission bars and firing the striker bar into the incident bar. A stress wave will travel through the incident bar in a one-dimensional fashion (if the bars are sufficiently long); upon reaching the sample, part of the incident stress wave will be reflected back into the incident bar and part of the incident stress wave will be transmitted through the sample into the transmission bar. This phenomenon occurs because of a mechanical impedance mismatch between the sample and the bars and is well documented in literature. The incident, reflected, and transmitted stress waves are then used to deduce the sample’s mechanical response by using one-dimensional wave propagation theory. The Kolsky bar has also been used in various configurations to conduct dynamic fracture experiments. A modified version used to conduct dynamic fracture initiation toughness experiments is described below.

A standard Kolsky bar with a nominal incident bar length, L_I , of 305 cm and nominal transmission bar length, L_T , of 149 cm was modified to accept a double impact tup and double support to facilitate the four point bending in the sample region. Machine drawings of the impact tup and support are provided in Appendix C. Both bars are nominally 19 mm in diameter and manufactured from C350 martensitic aging steel. A schematic of the setup is shown in Figure 3.4.

Strain gauges were placed at 232.1 cm and 44.5 cm from the sample ends of the incident

Figure 3.2: Four point bend fixture, sample, and microscope camera.

Figure 3.3: Digital microscope monitoring fatigue crack growth.

Figure 3.4: Schematic of modified Kolsky bar.

and transmission bars, respectively. The strain signals were used to determine the loading time history on the sample and to verify dynamic equilibrium during the experiment.

Annealed copper pulse shapers [19, 20] were used to generate ramp incident pulses. When impacted by the striker, the copper disk flows plastically, which increases its diameter and allows the striker momentum to transfer through the disk into the incident bar creating a ramp-like stress pulse with increasing amplitude. With proper selection of thickness and diameter of the pulse shaper and striker velocity magnitude, the shape of the increasing ramp stress pulse can be controlled. In this set of experiments the stress pulse was near linear. A ramp pulse was chosen because we wish to have a constant mode I stress intensity factor rate, $\dot{K}_I$. Because the equation used to calculate the stress intensity factor (Equation 3.1) is essentially a constant times the load, by making the load linearly increasing we can ensure that $\dot{K}_I$ will be linearly increasing as well. The copper pulse shapers, by lengthening the rise-time of the incident stress wave, also allow the sample to come into dynamic equilibrium before the crack initiates. If the crack were to initiate before the sample is in equilibrium then we would not be able to use quasi-static analysis to calculate the stress intensity factor. Stress equilibrium will be discussed further in Section 3.6.

3.5 Crack Initiation Time Detection

The most important measurement in dynamic crack initiation toughness testing is the crack initiation time. In quasi-static tests the stress intensity factor gradually increases at the crack tip over a very long period of time (e.g., minutes); the crack initiates and the load generally falls off very sharply allowing the experimentalist to easily detect the value of K_{Ic} directly from the load history without the need for special fiduciary timing tools to identify crack initiation. Furthermore, when the loading rate is quasi-static, the time-to-fracture, is on the order of 10^4 s and misdetection of the initiation by even several seconds will often lead to an undetectable difference in the reported value of K_{Ic} . However, we will see in our dynamic crack initiation experiments the time-to-fracture is on the order of 10^{-6} s and misdetection by even as little as 1 μ s can cause large differences in the reported value of K_{Ic} .

Several methods for detecting crack initiation were attempted in the course of this research, including using Vishay[®] Micro-Measurements[®] CD-02-10 single wire crack detection gages, a modified potential drop method for high rate crack propagation, and the use of a strain gage near the crack tip to detect the rise and fall of strain which signals unloading and crack initiation. The crack detection gages worked well when they stayed laminated to the surface of the sample; however, even though the Vishay[®] gages used a process of adhesion similar to the method for placing a strain gage on the sample, the gages tended to delaminate during the crack initiation process. This did not happen nearly as often when a strain gage was simply placed near or in front of the crack tip.

The potential drop method uses the knowledge that when a constant current is passed through a sample, a drop in the measured electric potential across the crack can be detected

by the crack advancement causing a resistance change in the sample. Using a modified method with a constant alternating current, it was discovered that an electrical potential drop could actually be detected when the two faces of the fatigue precrack simply opened, but before the crack initiated. This method showed promise, but in the end it was not used because of its need for sensitivity calibration and its general complication.

Crack initiation can be detected to a certain degree of accuracy by placing a strain gage near the crack tip and monitoring the strain. During loading the strain will increase and then drop off sharply when the crack initiates and the strain near the crack tip is relieved. The problem with this method is that the strain information takes time to propagate from the crack tip to the strain gages, which could cause a delay in the initiation detection time.

As a result of the knowledge gained by trying these other methods it was finally decided to use a sacrificial strain gage placed directly in front of the crack tip as a crack detection gage. This was done because the strain gages rarely delaminated even when being torn in half by the advancing crack. To prepare the strain gage, any excess substrate extending outside of the outermost wire was cut away to allow the first wire along the edge of the gage to be placed as near the crack tip as possible. The gages were then placed in front of the crack under a microscope which resulting in the gages being on the order of ≈ 0.1 mm from the tip. Figure 3.5 shows the sacrificial strain gage on the surface of a precracked sample. The fatigue precrack is difficult to see, but the removal of the excess substrate is easily identified in the photograph. Figure 3.6 shows a sample that was broken; the relationship of the strain gage to the crack tip can be observed in this photograph.

By placing the strain gage directly in front of the crack tip, one can easily distinguish the time-to-fracture. The load on the sample increases causing large strain in front of the crack, then when the crack initiates it splits the strain gage in half, breaking the circuit within the gage. Figure 3.7 shows a typical measurement as viewed on the oscilloscope from the sacrificial strain gage. In order to ensure the integrity of each measurement, a post-test visual inspection was done of each sample. If the sacrificial strain gage was not seen to have cleanly split in half or any signs of delamination were indicated, the test was considered invalid and the data not recorded.

A simple algorithm was used to detect the exact point where the circuit was broken and this fiduciary mark was then adjusted to allow it to correspond with the other measurement signals that indicate the load on the sample. This adjustment procedure will be discussed in detail in Section 3.6.

Figure 3.5: Sacrificial strain gage placed near crack tip.

Figure 3.6: Strain gage post-fracture showing relation to fatigue precrack.

Figure 3.7: Typical signal from sacrificial strain gage.

3.6 Data Reduction

3.6.1 Wave Speed Calculation

The first step in valid data reduction for a Kolsky bar experiment is to have an accurate measure of the wave speed in the bars. This can be measured by removing the transmission bar from the Kolsky apparatus and striking the incident bar with a striker. The compressive stress wave imparted on the incident bar by the striker will travel down the bar to the free surface at the other end and reflect back as a tensile wave. By recording the time-of-arrival of both the incident and reflected waves at the incident bar strain gage, and knowing the length between the strain gage and the end of the bar, the bar wave speed can be accurately calculated.

The wave speed experiment described in the last paragraph was conducted for the Kolsky bar at Sandia National Laboratories. Since it is very difficult to detect the exact moment the stress wave arrives by inspection, a simple algorithm was written to search the compressive incident wave for the time when the amplitude of the strain (indicated by electric potential on the oscilloscope) reached 0.2 V. This time is indicated in Figure 3.8 as t_1 . There is nothing especially particular about the value 0.2 V other than the fact that it was larger in magnitude than any conceivable noise in the strain signal. The same search was done on the tensile wave for an amplitude of -0.2 V. This time is indicated in Figure 3.8 as t_2 . To remove any high-frequency noise from the strain gage signal that might influence the search

Figure 3.8: Wave speed calculation.

algorithm, the strain signal was first filtered with a 4-pole Butterworth low-pass filter with a cutoff frequency of 40 000 Hz. Measuring the length between the incident bar strain gage and the end of the bar, L_{Ig} , to be 2.3209 m, the wave speed in the bar was calculated with Equation 3.6.

$$c_b = \frac{2L_{Ig}}{t_2 - t_1} = \frac{2 \cdot 2.3209 \text{ m}}{1555 \mu\text{s} - 610 \mu\text{s}} \approx 4912 \text{ m/s} \quad (3.6)$$

3.6.2 Strain Conversion

In the following subsections, references will be made to measured strain, ε . The signal actually measured on the oscilloscope from the strain gages is electric potential and must be converted to strain. The incident and transmission bars in the Kolsky apparatus both use strain gages configured in a half Wheatstone bridge. The electric potential measurements are converted to strain with Equation 3.7.

$$\varepsilon = \frac{1}{2} \frac{V_{out}}{V_{in} \cdot GF} \quad (3.7)$$

Where, V_{out} is the electric potential measured on the oscilloscope, V_{in} is the electric potential applied across the strain gage, and GF is the gage factor of the strain gages. All gages used in these experiments were Vishay[®] Micro Measurements 1000 Ω gages from lot number K60FD13 with $GF = 2.06 \pm 0.3\%$ and $V_{in} = 28 \text{ V}$.

3.6.3 Force Equilibrium Verification

The next step for valid data reduction in a Kolsky bar experiment is to ensure that the sample is in dynamic stress equilibrium during the time of interest for the test. For dynamic crack initiation toughness tests it is required that the sample be in equilibrium before the crack initiates; otherwise, quasi-static equations would not be valid for data reduction. Once again, this is why copper pulse shapers are needed to lengthen the rise-time of the incident stress wave allowing the sample to equilibrate. In order to check for dynamic equilibrium, a “one-wave, two-wave” technique is used. This is a common method of analysis used to check equilibrium in a Kolsky bar experiment. This requires knowing the time-of-arrival of both the incident and reflected wave on the incident bar strain gage and also the time of arrival of the transmitted wave on the transmission bar strain gage. In a conventional Kolsky bar test, measurements of the distance between the incident bar strain gage and the end of the incident bar, L_{Ig} , the length of the sample, L_s , the distance between the end of the transmission bar and the transmission bar strain gage, L_{Tg} , and the sample wave speed, c_s , would be made. The time-of-arrival of the incident wave, t_I , is then chosen either by inspection or with a numerical algorithm and the time-of-arrival of the reflected wave, t_R , and the transmitted wave, t_T , can then be calculated with Equation 3.8 and Equation 3.9, respectively.

$$t_R = t_I + \frac{2L_{Ig}}{c_b} \quad (3.8)$$

$$t_T = t_I + \frac{L_{Ig} + L_{Tg}}{c_b} + \frac{L_s}{c_s} \quad (3.9)$$

The force on the end of the incident bar (and therefore applied to the incident side of the sample) is calculated with Equation 3.10.

$$P_1 = E_b A_b (\varepsilon_I + \varepsilon_R) \quad (3.10)$$

Where, E_b is the elastic (Young’s) modulus of the bar which is either known beforehand or calculated with Equation 3.11,

$$E_b = c_b^2 \rho_b \quad (3.11)$$

with ρ_b being the density of the bars, A_b is the cross-sectional area of the bars and ε_I and ε_R are the incident and reflected strain measures taken from the incident bar strain gage and indexed from the respective times-of-arrival, t_I and t_R . The force on the end of the transmission bar (and therefore applied to the transmission side of the sample) is calculated with Equation 3.12.

$$P_2 = E_b A_b \varepsilon_T \quad (3.12)$$

Where, ε_T is the transmitted strain measured on the transmission bar strain gage indexed from the time-of-arrival, t_T . P_1 and P_2 are then plotted against each other to check for dynamic equilibrium. If the two curves nearly overlap then the sample is said to be in equilibrium.

The analysis presented above assumes one-dimensional wave propagation through the sample. In the modified Kolsky bar experiments outlined in Section 3.4 the entire gage

Figure 3.9: Uncorrected force equilibrium.

section is modified to accept the incident impact tups and transmitter supports. In addition, the sample is not a cylinder, but a prismatic beam. Under these conditions one-dimensional wave propagation through the gage section is invalid. If the time-of-arrival of the transmitted stress wave is calculated as in Equation 3.9 there will be significant error when attempting to plot P_1 and P_2 to verify equilibrium. This is demonstrated in Figure 3.9, where the transmitted stress wave is delayed by approximately $35\text{ }\mu\text{s}$. In order to correct for this, an estimate of the time for the stress wave to propagate through the gage section was made. This was performed² by employing the Sandia National Laboratories Eulerian hydrocode CTH [25], which was used to model the wave propagation through a shortened incident bar, the gage section, and a shortened transmission bar. The incident bar was impacted by a striker at 8 m/s and three probe locations were placed at the incident side of the gage section, the crack tip location, and the transmission side of the gage section. These locations are labeled, p_3 , p_2 , and p_1 , respectively, and illustrated in Figure 3.10a. Figure 3.10 graphically illustrates the stress wave propagation through the gage section with snapshots of the compressive stress wave taken at appropriate times of interest. Only the compressive wave is shown for visual tractability, but there are many tensile reflections occurring at the different interfaces.

The probe locations were used to record the stress wave passing through these points. The goal of these numerical experiments was not an attempt to simulate any deflection or crack initiation in the sample or even to match the amplitudes of the stress waves. The only measure of interest taken from these simulations was the time of arrival of the stress

²Acknowledgment is respectfully given to Dr. Paul A. Taylor for his help in performing this analysis.

Figure 3.10: Compressive stress wave progression.

Figure 3.11: Pressure profiles from CTH simulation.

waves. The data recorded at the three probe locations is shown in Figure 3.11. The three times-of-arrival corresponding to the locations, p_1 , p_2 , and p_3 are indicated in Figure 3.11 as t_{p_1} , t_{p_2} , and t_{p_3} , respectively. The time-of-arrival t_{p_3} was found to be approximately 25 μs , t_{p_2} was found to be approximately 37 μs , and t_{p_1} was found to be 60 μs . If we define the time for the stress wave to propagate through the gage section to be Δt_g , it can be calculated using Equation 3.13

$$\Delta t_g = t_{p_1} - t_{p_3} \quad (3.13)$$

The delayed transmitted stress can now be corrected by replacing the last term in Equation 3.9 with Δt_g from Equation 3.13. This results in Equation 3.14.

$$t_T = t_I + \frac{L_{Ig} + L_{Tg}}{c_b} + \Delta t_g \quad (3.14)$$

Correcting the data shown in Figure 3.9 in this fashion results in the data shown in Figure 3.12.

The time-to-fracture, t_f , was also corrected and indexed with the incident and transmitted bar signals in a similar fashion. If we define Δt_{SG} as the time for the stress wave to propagate from the incident bar side of the gage section to the strain gage place near the crack tip at the center of the sample we have the following:

$$\Delta t_{SG} = t_{p_2} - t_{p_3} \quad (3.15)$$

Using Equation 3.15 we can calculate the time-of-arrival of the stress wave at the crack tip,

Figure 3.12: Corrected force equilibrium plot.

t_{t0} , using Equation 3.16.

$$t_{f0} = t_I + \frac{L_{Ig}}{c_b} + \Delta t_{SG} \quad (3.16)$$

When the crack tip strain gage signal is indexed with the stress wave times-of-arrival from the incident and transmission bar signals, the actual time-to-fracture can be overlayed with the force equilibrium plots. This is also illustrated in Figure 3.12. Consequently, it is shown in Figure 3.12 that the sample is within a reasonable state of equilibrium through the time-to-fracture, t_f ; this will be discussed in more detail in Section 3.7.

3.6.4 Sample Boundary Velocity

A measure of interest not typically reported in Kolsky bar experiments, but can be readily calculated, is the bar end velocity. In a Kolsky bar experiment, the incident bar end moves at a higher velocity than the end of the transmission bar. This is caused by the addition of the compressive incident wave and the tensile reflected stress wave. The difference in relative motion of the two bar ends causes the sample to deform. The reason the bar end velocities were of interest in these experiments was their use in providing boundary conditions for the numerical simulations to be described in Chapter 5. The velocities of the incident bar end and the transmission bar end, v_1 and v_2 , respectively are calculated using Equation 3.17 and Equation 3.18

$$v_1 = c_b (\varepsilon_I - \varepsilon_R) \quad (3.17)$$

$$v_2 = c_b \varepsilon_T \quad (3.18)$$

Where, of course, each respective strain measure is indexed from the appropriate time locations described in the preceding subsection.

3.6.5 Crack Length Measurement

The last measurement needed before calculating the dynamic crack initiation toughness is the crack length, a . This is easily measure after the samples have been broken by examining the length of the fatigue crack under a microscope. One method of doing this is by using a microscope with a translating stage and a digital readout that describes the stage displacement. Following ASTM E399 we take measurements at three locations along the crack face. One in the center, and two each corresponding to distances of approximately $1/3W$ for each face of the sample. These three measurements are averaged to come up the the crack length used in calculating K_{Ic} . All crack length measurements are shown in Table D.1 in Appendix D.

3.6.6 Stress Intensity Factor and Dynamic Crack Initiation Toughness

Finally, the stress intensity factor and dynamic crack initiation toughness were calculated. Essentially the same procedure is used as was described in the K -calibration for the fatigue precrack in Section 3.3. However, in dynamic tests the load P is now a function of time, $P(t)$. This time dependent load replaces the quasi-static value in Equation 3.4 resulting in the stress intensity factor being a function of time. Following the substitution of Equation 3.4 into Equation 3.2 and that result into Equation 3.1 the following equation is used to find the stress intensity factor as a function of time, $K_I(t)$:

$$K_I(t) = \frac{3dP(t)}{BW^2} \sqrt{\pi a} \cdot \beta \left(\frac{a}{W} \right) \quad (3.19)$$

where, all definitions for Section 3.3 hold. The dynamic crack initiation toughness, K_{Ic} is then found by evaluating Equation 3.19 at the time-to-fracture, t_f , as shown in Equation 3.20.

$$K_{Ic} = \frac{3dP(t_f)}{BW^2} \sqrt{\pi a} \cdot \beta \left(\frac{a}{W} \right) \quad (3.20)$$

3.7 Results and Discussion

Initially, 30 samples where prepared and fatigue precracked following the procedures in Section 3.2 and Section 3.3. Of these initially prepared samples about one-half were sacrificed evaluating the different techniques used to capture accurate time-to-fracture measurements.

The remaining samples were used to conduct dynamic fracture initiation toughness tests at 2 different loading rates. These resulted in 9 valid experiments, 4 at a nominal loading rate of $2.3 \times 10^6 \text{ MPa}\sqrt{\text{m/s}}$ and 5 at a nominal loading rate of $5.4 \times 10^6 \text{ MPa}\sqrt{\text{m/s}}$.

The nominal loading rates, expressed in terms of mode I stress intensity factor rate, $\dot{K}_I$, were calculated by dividing the average dynamic crack initiation toughness, K_{Ic} , by the average time-to-fracture t_f . Each of the two loading conditions were created by changing the gas gun pressure and the copper pulse shaper size in the Kolsky apparatus. The calculation gives a reasonable estimate of the loading rates without the need to curve fit because the rise time of the load was near linear.

Complete results from a typical test are shown in Figure 3.13. The raw data is shown in Figure 3.13a, just as observed on the oscilloscope. All of the other subfigures shown were processed as described in Section 3.6 after being digitally filtered with a 4-pole Butterworth low-pass filter with a cutoff frequency of 40 000 Hz. This was done to remove the very high frequency bit noise that overlays the strain signals and resulted in robust algorithms for detecting the stress wave times-of-arrival robust. The results from all tests are included in Appendix A and Appendix B.

It is shown in Figure 3.13d that the sample is in a state of dynamic force equilibrium through the time-to-fracture. After the crack initiates, sample equilibrium appears to diverge, but it is unknown if this is what is actually happening because the equilibrium calculation is done from the incident and transmission bar strain gages assuming a constant propagation of stress from the impacting tups and supports; after crack initiation the beam sample begins to slide along the supports and it is unknown how this phenomenon affects the stress wave propagation. However, since only the crack initiation toughness is the desired measurement, only force equilibrium through time-to-fracture is required.

Figure 3.13e shows the sample boundary velocities as a function of time. In a similar fashion to the force equilibrium plot, unknown boundary conditions after crack initiation cause uncertainty in the velocities after t_f .

Figure 3.13f shows the stress intensity factor as a function of time. To evaluate the crack initiation toughness the stress intensity factor is evaluated at the time-to-fracture. The stress intensity factor is shown to keep increasing after crack initiation in the plot; however, all stress intensity factor data to the right of the vertical line ($\forall t > t_f$) is invalid because at that point the crack length, a , is now increasing and the stress intensity factor becomes a function of the moving crack's speed, $\dot{a}$. This process is typically identified in literature as the crack growth toughness. Crack growth toughness is outside the scope of this research, therefore, crack speed was not measured.

Each sample was visually inspected post fracture to ensure that the crack detection strain gage was in place on each fractured beam sample half. If one side or both sides were not cohesively intact, the test was invalidated. Figure 3.14 shows the results from all the valid tests.

The nominal loading rate of $2.3 \times 10^6 \text{ MPa}\sqrt{\text{m/s}}$ was created by setting the Kolsky bar

(a) Raw data.

(b) Incident signal.

(c) Transmitted signal.

(d) Force equilibrium.

(e) Sample boundary velocity.

(f) Stress intensity factor.

Figure 3.13: Results from a typical dynamic crack initiation toughness test using the modified Kolsky bar.

Figure 3.14: Dynamic crack initiation toughness as a function of loading rate.

gas gun pressure to 275.79 MPa and using an annealed copper pulse shaper of 1.32 mm thickness by 7.33 mm diameter. At this loading rate, the experiments showed excellent repeatability with all of the tests resulting in a dynamic crack initiation toughness value of approximately 65 MPa√m. The time-to-fracture value for this nominal loading rate was approximately 27 μs for each test. The K_{Ic} value of approximately 65 MPa√m is roughly what the reported quasi-static value is for 4340 steels with approximately the same heat treatment. This implies that at this nominal loading rate there is no difference between the quasi-static and dynamic crack initiation toughness. The second nominal loading rate of 5.3×10^6 MPa√m/s was produced by using a Kolsky apparatus gas gun pressure of 413.69 MPa and an annealed copper pulse shaper of 1.32 mm thickness by 8.33 mm diameter. At this loading rate the experiments were less reproducible with dynamic crack initiation toughness values ranging from 139 MPa√m to 165 MPa√m and time-to-fracture measurements ranging from 25 μs to 32 μs. The actual loading rates in this range were from 4.34×10^6 MPa√m/s to 6.32×10^6 MPa√m/s. It was noticed that the measured values of dynamic crack initiation toughness were much higher at the higher nominal loading rate.

3.8 Camera Data

A subset of dynamic crack initiation toughness experiments were conducted on a similar modified Kolsky bar at Purdue University. The sample preparation for these experiments was not as well controlled as the experiments reported above. These experiments were done

to initially evaluate the viability of conducting controlled loading experiments in the Kolsky apparatus. For this reason, the samples were not machined or heat treated to the tolerances reported in Section 3.2, and are not included as valid test data in Figure 3.14. However, the experiments initially conducted at Purdue did include the use of a Cordin high-speed rotating mirror camera. The Cordin camera at Purdue has 32 charge-coupled devices (CCDs) capable of frame rates up to 2 million frames per second. The desire in these experiments was to capture the entire event from the onset of loading, through crack initiation and propagation. In order to capture the desired events the camera was run at a nominal frame rate of 250 000 frames per second resulting in a total recording time of approximately 128 μ s. With a sample period of roughly 4 μ s the frame rate was not fast enough to accurately resolve time-to-fracture measurements; therefore, the camera was ultimately abandoned, but does offer some qualitative comparisons that will be used in Chapter 5 to compare against simulation results. More images will be shown in those comparisons, but Figure 3.15 offers a view of a single frame taken from the Cordin camera just after crack initiation in one of the tests.

3.9 Scanning Electron Microscopy

A selection of fractured samples were taken to the lab for scanning electron microscope (SEM) imaging. This was done to evaluate any microstructural differences that may account for, or explain the loading rate dependence of, the measured values of crack initiation toughness. One might expect that for the crack initiation toughness to be higher at one loading rate could be a result of an increase in ductility at the crack tip. One hypothesis proposed was that this increase in ductility was caused by adiabatic heating in the crack tip plastic zone. However, the SEM images shown in Figure 3.16 at the two different nominal loading rates does not show any evidence to confirm this hypothesis. Both images were taken at a magnification of 1500X at a location very near the crack initiation in what most fracture analysts would call the process zone. Even to the untrained eye, it is easy to see that neither image shows a distinguishable difference from the other. One might expect to see much larger voids or evidence of void coalescence if more ductility were occurring due to adiabatic heating.

3.10 Concluding Remarks

This chapter describes in detail the design of a dynamic crack initiation toughness specimen, the fatigue cracking process, a method for experimentally capturing the time-to-fracture, a novel experimental technique for capturing dynamic crack initiation toughness, and the complete method of data reduction. We also reported values of dynamic crack initiation toughness for a 4340 steel specimen at two different near constant nominal loading rates.

A future iteration of this experimental procedure might attempt to either design the sample smaller to fit within the diameter of the incident and transmission bars or possibly

Figure 3.15: Single frame from Cordin camera taken after crack initiation.

use larger diameter bars; if the impacting tups and supports could be embedded directly in the end of the bars, it would minimize the departure from one dimensional wave propagation and perhaps eliminate the need for the special procedure that corrects the timing for the two dimensional wave propagation that manifests in this design. Both of these suggestions cause additional difficulties that would have to be overcome in order for the experiment to be valid. If the sample is too small the crack tip plastic zone may interfere with the boundaries causing the measure of K_{Ic} to be invalid because the idea of small scale yielding will not hold. Making bars with diameters large enough to embed the impacting tups and supports in the ends may require that the bars be very long for one dimensional wave propagation to be valid. Very long, large diameter bars are difficult and expensive to machine and supporting them in a fashion that minimizes friction can also be very difficult.

Additional work should also be put into accurately capturing the time-to-fracture measurement. This is possibly the most important measurement in the dynamic crack initiation

(a) $2.36 \times 10^6 \text{ MPa}\sqrt{\text{m/s}}$ nominal loading rate.

(b) $5.3 \times 10^6 \text{ MPa}\sqrt{\text{m/s}}$ nominal loading rate.

Figure 3.16: SEM image taken from fracture surface initiation point.

toughness process yet is typically skipped over in literature as a trivial exercise. The potential drop method briefly described earlier could possibly be the best way to capture this measurement. It has been well established for fatigue crack measurements and could possibly be extended to measure not only the crack initiation time but also crack propagation at high loading rates with further research.

4 Viscoplasticity Using Peridynamics

4.1 Introduction

The culmination of the work reported in the preceding chapter are the results published in Figure 3.14 showing a rate dependence of the dynamic crack initiation toughness for a 4340 steel. A minimal amount of investigation was done at the microstructural level to look for clues which might explain the rate dependence. A material scientist might undertake a more thorough investigation looking at grain size effects, additional scanning electron microscopy, and transmission electron microscopy. As engineers, we will simply make use of the knowledge that the steel exhibits a rate dependence without further investigation into the microstructural evolution and mechanics. Using the knowledge of rate dependent crack initiation, we will attempt to develop simulations at the continuum level which result in similar observations as the experiments.

We will start by choosing an appropriate constitutive model and implementing it the peridynamic framework. The peridynamic theory of solid mechanics was introduced in Section 1.2. To date, only material models with severe restrictions such as the $1/4$ Poisson's ratio artifact, also discussed in Section 1.2 have been utilized within this framework. It has been demonstrated that peridynamics has many positive features for modeling failure due to its lack of dependence on spacial derivatives. We choose to implement a rate sensitive plasticity model into the peridynamic framework in order to take advantage of the straightforward ability to capture material failure and still model deformations in a more realistic sense. A viscoplastic model was chosen because of the desire to model both rate dependence and strain hardening of the material. The model is implemented by taking a classic (stress-strain) model and converting it to be used with peridynamic force-vector states. We adopt this approach as a convenience to avoid having to hypothesize and test a constitutive model formulated exclusively in terms of force-vector states. This chapter explains how the constitutive model was implemented into the peridynamic framework and then validates the model with experimental data. A great deal of the information presented in this chapter is published in Foster et al. [15].

4.2 Peridynamic Kinematics

The first step in numerically implementing a traditional (formulated in terms of stress and strain) constitutive model into the state-based peridynamic framework is finding an approximation to the local deformation gradient, $\mathbf{F}$, for each node. Recall from classical continuum mechanics that the deformation gradient is defined by Equation 4.1

$$\mathbf{F} = \mathbf{I} + \mathbf{u}\nabla_{\mathbf{x}}^1 \quad (4.1)$$

where $\mathbf{I}$ is the identity tensor and $\nabla_{\mathbf{x}}$ is the gradient operator with respect to $\mathbf{x}$ in the reference configuration. In order for $\mathbf{F}$ to be defined, all of the partial derivatives contained in $\mathbf{u}\nabla_{\mathbf{x}}$ must exist. This requires the displacement field to be continuously differentiable. In other forms of computational mechanics (e.g., Finite Element Method) these partial derivatives must only be defined in a weak sense in order for $\mathbf{F}$ to exist; however, we will not make this restriction in the peridynamic formulation [3]. We will use the true deformation, defined by a deformation-vector state $\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle$ (Equation 4.2), to approximate $\mathbf{F}$

$$\underline{\mathbf{Y}}[\mathbf{x}, t]\langle\boldsymbol{\xi}\rangle = \boldsymbol{\xi} + \boldsymbol{\eta} \quad (4.2)$$

where $\boldsymbol{\xi}$ is the relative position between two material points

$$\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x} \quad (4.3)$$

and $\boldsymbol{\eta}$ is the relative displacement,

$$\boldsymbol{\eta} = \mathbf{u}[\mathbf{x}', t] - \mathbf{u}[\mathbf{x}, t] \quad (4.4)$$

$\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle$ is a vector function that associates any bond $\boldsymbol{\xi}$ with the deformed image of the bond. Figure 4.1 illustrates the key differences between $\mathbf{F}$ and $\underline{\mathbf{Y}}$. Because $\mathbf{F}$ is a second order tensor it is only capable of mapping a circle into an ellipse (sphere into an ellipsoid in three dimensions), whereas, $\underline{\mathbf{Y}}$ is capable of mapping a circle into any conceivable shape and includes discontinuous deformations or even replacement, as shown by the reversal of material at locations $\mathbf{A}$ and $\mathbf{B}$ in Figure 4.1b.

To approximate the deformation gradient from the true deformation via the deformation vector-state we start by defining a non-local *shape tensor* with the following integral:

$$\mathbf{K}[\mathbf{x}, t] = \int_{\mathcal{H}} \omega(|\boldsymbol{\xi}|) (\boldsymbol{\xi} \otimes \boldsymbol{\xi}) dV_{\mathbf{x}'} \quad (4.5)$$

where $\otimes$ is the dyadic product operator, and ω is defined as an *influence function*, which is scalar valued and dependent on $|\boldsymbol{\xi}|$. In this implementation, ω is always either 0 or 1, which corresponds to whether the bond is “broken” or not. Broken bonds are the method in which material failure is introduced in the peridynamic theory, and while this is one of the primary advantages of the theory its discussion will be postponed until Chapter 5. ω could

¹ $F_{ij} = \delta_{ij} + \frac{\partial u_i}{\partial x_j}$ using indicial notation.

(a) Deformation gradient.

(b) Deformation vector-state.

Figure 4.1: Illustration of key difference between deformation gradient and deformation vector-state.

also be used as a distributable influence function where certain material neighbors have more influence than others. To date, only constant influence functions have been studied with no apparent negative effects (instabilities, etc.) The integral in Equation 4.5 results in a positive definite tensor when evaluated; therefore, $\mathbf{K}$ will always be invertible. For a discrete system, we can represent the non-local shape tensor for a node with the following sum:

$$\mathbf{K}[\mathbf{x}_i, t] \approx \sum_{j=1}^k \omega(|\boldsymbol{\xi}|) (\boldsymbol{\xi} \otimes \boldsymbol{\xi}) V_j \quad (4.6)$$

where $\boldsymbol{\xi}$ is now

$$\boldsymbol{\xi} = \mathbf{x}_j - \mathbf{x}_i \quad (4.7)$$

It can likewise be shown that the discrete $\mathbf{K}$ in Equation 4.6 will be invertible as long as three non-coplanar vectors $\boldsymbol{\xi}$ are used in the formulation.

Knowing the shape tensor, the approximated deformation gradient, $\mathbf{F}$, at a material point $\mathbf{x}$ is given by Equation 4.8.

$$\mathbf{F}[\mathbf{x}, t] = \left[\int_{\mathcal{H}} \omega(|\boldsymbol{\xi}|) (\underline{\mathbf{Y}} \langle \boldsymbol{\xi} \rangle \otimes \boldsymbol{\xi}) dV_{\mathbf{x}'} \right] \mathbf{K}^{-1} \quad (4.8)$$

Similarly, in discrete form:

$$\mathbf{F}[\mathbf{x}_i, t] \approx \left[\sum_{j=1}^k \omega(|\boldsymbol{\xi}|) (\underline{\mathbf{Y}} \langle \boldsymbol{\xi} \rangle \otimes \boldsymbol{\xi}) V_j \right] \mathbf{K}^{-1} \quad (4.9)$$

The deformation gradient can be shown to be exact for a constant deformation. This is always true irrespective of the location of a material point within a body, even along boundaries or near discontinuities. If we assume a constant deformation-vector state, $\underline{\mathbf{Y}}_i = F_{ip} \xi_p$, then the proof follows:

$$\begin{aligned} F_{ij} &= \left[\int_H \omega(\xi) F_{ip} \xi_p \xi_k dV_{\xi} \right] K_{kj}^{-1} \\ &= F_{ip} \left[\int_H \omega(\xi) \xi_p \xi_k dV_{\xi} \right] K_{kj}^{-1} \\ &= F_{ip} K_{pk} K_{kj}^{-1} \\ &= F_{ip} \delta_{pj} \\ &= F_{ij} \end{aligned}$$

With the deformation gradient in hand, the rest of the kinematics follow the standard definitions laid out in many texts. Included here for completeness, will be the foundation used to find the *unrotated rate of deformation tensor*, $\mathbf{d}$. First, the velocity gradient tensor is given by Equation 4.10.

$$\mathbf{L} = \dot{\mathbf{F}} \mathbf{F}^{-1} \quad (4.10)$$

Since $\mathbf{F}$ is defined in material (Lagrangian) coordinates, $\dot{\mathbf{F}}$ is the material time derivative of $\mathbf{F}$. The velocity gradient can be decomposed into symmetric and skew-symmetric parts. The symmetric part is referred to as the rate of deformation tensor and is shown in Equation 4.11.

$$\mathbf{D} = \frac{1}{2} [\mathbf{L} + \mathbf{L}^T] \quad (4.11)$$

If the polar decomposition theorem is applied to $\mathbf{F}$, we have

$$\mathbf{F} = \mathbf{V} \mathbf{R} = \mathbf{R} \mathbf{U} \quad (4.12)$$

where $\mathbf{R}$ is a orthogonal tensor describing a rigid body rotation. The tensor $\mathbf{R}$ is calculated in the incremental formulation outlined by Taylor and Flanagan [14]. $\mathbf{V}$ and $\mathbf{U}$ are the left and right stretch tensors, respectively. Now we can use the right polar decomposition from Equation 4.12 and substitute it into Equation 4.10 to define the velocity gradient in the following way:

$$\mathbf{L} = \dot{\mathbf{R}} \mathbf{R}^T + \mathbf{R} \dot{\mathbf{U}} \mathbf{U}^{-1} \mathbf{R}^T \quad (4.13)$$

where we have made use of the fact that $\mathbf{R}^{-1} = \mathbf{R}^T$ for orthogonal tensors. The term $\dot{\mathbf{R}} \mathbf{R}^T$ in Equation 4.13 is skew symmetric and represents a rate of rotation. The symmetric part of $\dot{\mathbf{U}} \mathbf{U}^{-1}$ is referred to as the unrotated rate of deformation tensor. Equating with Equation 4.11, the unrotated rate of deformation tensor can be described as shown in Equation 4.14.

$$\mathbf{d} = \frac{1}{2} [\dot{\mathbf{U}} \mathbf{U}^{-1} + \mathbf{U}^{-1} \dot{\mathbf{U}}] = \mathbf{R}^T \mathbf{D} \mathbf{R} \quad (4.14)$$

4.3 Principal of Material Frame Indifference

The Principal of Material Frame Indifference (also referred to as objectivity) states that a constitutive law must be invariant to a change of observer reference frame in the absence of external fields, such as magnetic fields, that would define a preferred direction in space. Therefore, only objective quantities can be used in a constitutive equation. For this reason we will formulate our constitutive relationship involving the Cauchy stress in the unrotated configuration. The reason for this choice will be made clear in the following paragraphs. The unrotated Cauchy stress, $\boldsymbol{\tau}$, is related to the rotated Cauchy stress or true stress, $\boldsymbol{\mathcal{T}}$, with the rotation tensor $\mathbf{R}$ by the following:

$$\boldsymbol{\tau} = \mathbf{R}^T \boldsymbol{\mathcal{T}} \mathbf{R} \quad (4.15)$$

Because numerical techniques require the integration of constitutive equations involving the stress rate, we require that the stress rate be objective. Johnson and Bammann [35] building on the work of Green and Naghdi [23], showed if a motion is considered that differs from a given motion only by a superimposed rigid body motion, i.e.,

$$\mathbf{z}^* = \mathbf{a}(t) + \mathbf{M}(t) \mathbf{z} \quad (4.16)$$

where $\mathbf{a}$ is a vector function of t that can be interpreted as a rigid body translation and $\mathbf{M}$ is a proper orthogonal tensor function of t that can be interpreted as a rotation, when the motion prescribed in Equation 4.16 is applied to the unrotated and rotated Cauchy stress rate tensors, the following results:

$$\dot{\boldsymbol{\tau}}^* = \dot{\boldsymbol{\tau}} \quad (4.17)$$

$$\dot{\boldsymbol{\mathcal{T}}}^* = \dot{\mathbf{M}} \boldsymbol{\mathcal{T}} \mathbf{M}^T + \mathbf{M} \dot{\boldsymbol{\mathcal{T}}} \mathbf{M}^T + \mathbf{M} \boldsymbol{\mathcal{T}} \dot{\mathbf{M}}^T \quad (4.18)$$

From Equations 4.17 and 4.18 it is clear that the unrotated Cauchy stress rate is objective whereas the Cauchy stress rate in the rotated configuration is not. In the subsequent sections describing our implementation of the constitutive model, all stress quantities will be assumed to be in the unrotated configuration to ensure compliance with the Principal of Material Frame Indifference.

4.4 Stress to Peridynamic State Conversion

If we assume the unrotated Cauchy stress tensor is a known quantity we can rotate back into the deformed configuration using the rotation tensor from the polar decomposition as follows:

$$\boldsymbol{\mathcal{T}} = \mathbf{R} \boldsymbol{\tau} \mathbf{R}^T \quad (4.19)$$

We can now convert the rotated Cauchy stress tensor into the first Piola-Kirchhoff stress tensor, $\boldsymbol{\sigma}$, with the relationship

$$\boldsymbol{\sigma} = \det(\mathbf{F}) \boldsymbol{\mathcal{T}} \mathbf{F}^{-T} \quad (4.20)$$

and the first Piola-Kirchhoff stress tensor can be converted into the force-vector state with the following relationship² [59]:

$$\underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle = \omega(|\boldsymbol{\xi}|) \boldsymbol{\sigma} \mathbf{K}^{-1} \boldsymbol{\xi} \quad (4.21)$$

The force-vector state, $\underline{\mathbf{T}}\langle \boldsymbol{\xi} \rangle$, can then be substituted back into Equation 1.5 and numerically integrated to find the displacements at the next time step. Then the process is repeated for the desired number of time steps to get a final solution. This method is purely meshless Lagrangian in that it produces all spatial information (displacement, velocity, acceleration, stress, strain) at each node for each time step without the need for Gauss integration points and interpolation of nodal values.

4.5 von Mises Plasticity

Data used to determine constitutive model parameters is usually collected during a uniaxial tension test. We need a way to use this information to model arbitrary deformations. The theory we adopt here is well developed in many texts [26, 42] and is commonly referred to as

²The full derivation of this relationship is included in Appendix F

von Mises plasticity theory. It has been observed experimentally that, as a first approximation, metals yield as a result of shear deformations (independent of hydrostatic pressure). If this assumption of pressure independence is valid, it follows that yielding depends only on the deviatoric stress, which is defined in Equation 4.22

$$\mathbf{S} = \boldsymbol{\tau} - \frac{1}{3}\text{tr}(\boldsymbol{\tau})\mathbf{I} \quad (4.22)$$

where $\boldsymbol{\tau}$ is the unrotated Cauchy stress tensor and $\text{tr}(\boldsymbol{\tau}) = \tau_{11} + \tau_{22} + \tau_{33}$ and $\mathbf{I}$ is the identity tensor. The second term in Equation 4.22 represents the hydrostatic pressure, and by subtracting it from the Cauchy stress only the stress as a result of shear deformation is left. If we assume that the state of stress as measured during a uniaxial tension test at the onset of yielding is defined by a stress, G , then it follows,

$$\boldsymbol{\tau} = \begin{bmatrix} G & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (4.23)$$

the deviatoric stress tensor corresponding to this state of stress is defined by

$$\mathbf{S} = \begin{bmatrix} \frac{2}{3}G & 0 & 0 \\ 0 & -\frac{1}{3}G & 0 \\ 0 & 0 & -\frac{1}{3}G \end{bmatrix} \quad (4.24)$$

and the magnitude³ of the deviatoric stress tensor is defined as

$$S = |\mathbf{S}| = \sqrt{\frac{2}{3}}G \quad (4.25)$$

The term $\sqrt{2/3}G$ represents the extent of the yield surface in stress space. Stress space is a three-dimensional space where the axes represent the principal stresses. In von Mises plasticity theory the yield surface is always a cylinder with the central axis along the hydrostat, defined by the line $\sigma_I = \sigma_{II} = \sigma_{III}$, where σ_I , σ_{II} , and σ_{III} are the principal stresses. A state of stress can never be outside the yield surface, but can sit on the yield surface indefinitely, and the yield surface can change in size, depending on G .

Once the value of the deviatoric stress magnitude has exceeded G the material is said to be yielded and deforms according to the *flow rule*, which describes the plastic deformation. To begin the discussion of the flow rule, we will define the total (unrotated) deviatoric strain rate to be as follows:

$$\dot{\mathbf{e}} = \mathbf{d} - \frac{1}{3}\text{tr}(\mathbf{d})\mathbf{I} \quad (4.26)$$

We will assume that the total deviatoric strain rate, $\dot{\mathbf{e}}$, can be additively decomposed into purely elastic and plastic parts as shown in Equation 4.27.

$$\dot{\mathbf{e}} = \dot{\mathbf{e}}^e + \dot{\mathbf{e}}^p \quad (4.27)$$

³The magnitude of a tensor $\mathbf{A}$ is defined by $|\mathbf{A}| = \sqrt{A_{ij}A_{ij}}$ using Einstein indicial summation.

We assume that the elastic part, $\dot{\mathbf{e}}^e$, is fully recoverable and the plastic part, $\dot{\mathbf{e}}^p$, results in permanent strain. The elastic part of the deviatoric strain rate tensor can then be written according to Hooke's law for stress and strain rates as follows:

$$\dot{\mathbf{e}}^e = \frac{\dot{\mathbf{S}}}{2\mu} \quad (4.28)$$

where μ is the shear modulus. In order to define the plastic part of the deviatoric strain rate tensor we will assume a flow rule of the form:

$$\dot{\mathbf{e}}^p = \dot{\lambda} \mathbf{Q} \quad (4.29)$$

where $\dot{\lambda}$ is a yet undetermined scalar and $\mathbf{Q}$ is a unit tensor in the direction of deviatoric stress defined in Equation 4.30.

$$\mathbf{Q} = \frac{\mathbf{S}}{S} \quad (4.30)$$

Equation 4.29 is called an *associated* flow rule because the direction of plastic flow is associated with the direction of deviatoric stress. This is one of the most common flow rules and is almost always used to model plasticity in metals that deform with pressure invariance.

4.6 Yield Surface Determination

At each time step and for each peridynamic node, we must calculate the scalar value representing the extent of the yield surface. If we assume a yielded stress magnitude, G , that is defined as a function of *equivalent plastic strain* and its time derivative *equivalent plastic strain rate* (ε^p and $\dot{\varepsilon}^p$, respectively), or in notational form:

$$G = f(\varepsilon^p, \dot{\varepsilon}^p) \quad (4.31)$$

In order to define G at a time, t , in our numerical solution scheme, we must decide which values of ε^p and $\dot{\varepsilon}^p$ to use. The most straightforward method is to use a backward explicit scheme which defines G as in Equation 4.32:

$$G_t = f\left(\varepsilon_{t-\Delta t}^p, \frac{\varepsilon_{t-\Delta t}^p - \varepsilon_{t-2\Delta t}^p}{\Delta t}\right) \quad (4.32)$$

where Δt is a constant time step increment. The constant time step assumption is used here to keep the notation tractable, but in general is not a requirement. While this is a straightforward method for defining G_t , stability calculations performed by Silling [55] have shown this method to be unstable for all but trivial cases. A different approach was determined by the same stability calculations to be stable without additional restriction on time step size beyond that for traditional explicit finite differencing methods. This approach is adopted here and is a backward implicit definition of the form:

$$G_t = f\left(\varepsilon_{t-\Delta t}^p, \frac{\varepsilon_t^p - \varepsilon_{t-\Delta t}^p}{\Delta t}\right) \quad (4.33)$$

Here, G_t is implicit in ε_t^p and therefore not a straightforward a calculation. The following steps describe how we will solve for G_t by casting the problem in a framework involving only scalars for simplicity. First, we will define the equivalent plastic strain rate, $\dot{\varepsilon}^p$, to be

$$\dot{\varepsilon}^p = \sqrt{\frac{2}{3}} |\dot{\mathbf{e}}^p| \quad (4.34)$$

The $\sqrt{2/3}$ term appears by convention similar to that which results in Equation 4.25 because $\dot{\varepsilon}^p$ is the plastic strain rate that would be measured in a uniaxial tension test. If we substitute Equation 4.29 into Equation 4.34, remembering that $\mathbf{Q}$ is a unit tensor we have the following:

$$\dot{\varepsilon}^p = \sqrt{\frac{2}{3}} \dot{\lambda} \quad (4.35)$$

Now we define a scalar, $\dot{e}$, which is the projection of the total deviatoric strain rate tensor in the direction of deviatoric stress we have⁴:

$$\dot{e} = \dot{\mathbf{e}} : \mathbf{Q} \quad (4.36)$$

where, $:$ is the tensor dot product operator. Now we apply a similar relationship to $\dot{\mathbf{e}}^e$

$$\dot{e}^e = \dot{\mathbf{e}}^e : \mathbf{Q} \quad (4.37)$$

If we combine Equations 4.29, 4.36, and 4.37 with Equation 4.27, we have the relationship that follows:

$$\dot{e} = \dot{e}^e + \dot{\lambda} \quad (4.38)$$

Substituting Equation 4.28 into Equation 4.37 we find that the magnitude of elastic deviatoric strain rate can be described as shown in Equation 4.39.

$$\dot{e}^e = \frac{\dot{S}}{2\mu} \quad (4.39)$$

where $\dot{S}$ is the time derivative of the deviatoric stress magnitude, $S = |\mathbf{S}|$. Next we substitute Equation 4.39 into Equation 4.38 and multiply the result by Δt in order to convert the rate terms into increments, which results in the following:

$$\Delta e = \frac{\Delta S}{2\mu} + \Delta \lambda \quad (4.40)$$

If we assume that Δt represents a time increment between times t and $t - \Delta t$, we can expand the deviatoric strain increment and slightly rearrange Equation 4.40 to provide Equation 4.41,

$$\Delta e_{t-\Delta t/2} - \frac{S_t - S_{t-\Delta t}}{2\mu} - \Delta \lambda_{t-\Delta t/2} = 0 \quad (4.41)$$

Assuming the material is yielded at the time t , we can substitute Equation 4.25 into Equation 4.41 to have:

$$\Delta e_{t-\Delta t/2} - \frac{\sqrt{2/3} G_t - S_{t-\Delta t}}{2\mu} - \Delta \lambda_{t-\Delta t/2} = 0 \quad (4.42)$$

⁴ $\mathbf{A} : \mathbf{B} = A_{ij} B_{ij}$

If we multiply Equation 4.35 by Δt to once again convert rates into increment values, we can substitute the result into Equation 4.33 to redefine our yield function as follows:

$$G_t = f \left(\varepsilon_{t-\Delta t}^p, \sqrt{\frac{2}{3}} \frac{\Delta \lambda_{t-\Delta t/2}}{\Delta t} \right) \quad (4.43)$$

Finally we substitute Equation 4.43 into Equation 4.42 to get

$$\Delta e_{t-\Delta t/2} - \Delta \lambda_{t-\Delta t/2} - \frac{1}{2\mu} \left[\sqrt{\frac{2}{3}} f \left(\varepsilon_{t-\Delta t}^p, \sqrt{\frac{2}{3}} \frac{\Delta \lambda_{t-\Delta t/2}}{\Delta t} \right) - S_{t-\Delta t} \right] = 0 \quad (4.44)$$

Equation 4.44 involves only terms that are defined from the previous time step $t - \Delta t$, except for $\Delta \lambda$, which can be solved with a numerical root solver. If the left-hand side (LHS) of Equation 4.44 is continuous, it can be differentiated with respect to $\Delta \lambda$ therefore, a Newton-Raphson method can be used if desired. However, the LHS of Equation 4.44 is a monotonically decreasing function of $\Delta \lambda$, and as $\Delta \lambda \rightarrow 0$, the slope of this function becomes infinity and Newton's method will not converge. A notional curve representing the LHS of Equation 4.44 as a function of $\Delta \lambda$ is presented in Figure 4.2 to illustrate this idea. Therefore, for the simulations that will be shown in subsequent sections, a bisection method was used to solve for $\Delta \lambda$. Generally, $\Delta \lambda$ is a very small positive number much less than 1. Therefore, the root was assumed to be $0 < \Delta \lambda < 1$ and has converged in all test cases. Perhaps a numerical root solver such as Brent's Method would be the most efficient algorithm to use because it guarantees convergence if the root is bounded and also converges faster than the bisection method alone, but we found the bisection method to be sufficient for our purposes.

Once $\Delta \lambda$ is known, the current value of the yield surface, G_t , can be found by substituting $\Delta \lambda$ into the relationship shown in Equation 4.43.

4.7 Evaluation of Stress Tensor

Once G_t is known, we can decide whether a node has yielded or not by comparing the magnitude of the deviatoric stress with the scalar value indicating the extent of the yield surface. First we assume a "trial" deviatoric stress by considering only an elastic deformation increment across a time step as follows:

$$\mathbf{S}_t^{tr} = \mathbf{S}_{t-\Delta t} + 2\mu \Delta \mathbf{e}_{t-\Delta t/2} \quad (4.45)$$

Now we can define the deviatoric stress at a time step, t , according to the following:

$$\mathbf{S}_t = \begin{cases} \mathbf{S}_t^{tr} & |\mathbf{S}_t^{tr}| < \sqrt{2/3} G_t \\ \sqrt{2/3} G_t \mathbf{Q}_t^{tr} & |\mathbf{S}_t^{tr}| \geq \sqrt{2/3} G_t \end{cases} \quad (4.46)$$

Geometrically, the second part of Equation 4.46 represents a "radial return to the yield surface," which ensures that any stress state lies within or on the yield surface for all time.

Figure 4.2: Notional curve for $\Delta\lambda$ root.

With the new deviatoric stress tensor we can easily find the new value of Cauchy stress as shown in Equation 4.47

$$\boldsymbol{\tau}_t = \mathbf{S}_t + p_t \mathbf{I} \quad (4.47)$$

where p_t is the updated hydrostatic pressure defined by the equation

$$p_t = p_{t-\Delta t} + \mathcal{K} \text{tr}(\mathbf{d}_{t-\Delta t/2}) \Delta t \quad (4.48)$$

and $\mathcal{K}$ is the material's bulk modulus.

4.8 Evaluation of Equivalent Plastic Strain

Once a stress tensor is known in time t , the only remaining operation in this time step is to find the updated value of equivalent plastic strain. The most straightforward method of evaluating equivalent plastic strain would be to simply substitute the value of $\Delta\lambda$ into the differenced form of Equation 4.35 and solve for the equivalent plastic strain at time t . A more general form will be used because, in cases where G_t is not dependent on $\dot{\epsilon}^p$, the value of $\Delta\lambda$ does not have a physical meaning. However, the equivalent plastic strain can change over a time step through mechanisms other than rate dependence. If we assume a scalar value of deviatoric plastic strain is defined in a similar fashion to the elastic and total deviatoric strains defined earlier, we have:

$$\dot{e}^p = |\dot{\mathbf{e}}^p| = \dot{\mathbf{e}}^p : \mathbf{Q} \quad (4.49)$$

If we solve Equation 4.27 for $\dot{\epsilon}^p$ and substitute into Equation 4.49, we have

$$\dot{\epsilon}^p = (\dot{\epsilon} - \dot{\epsilon}^e) : \mathbf{Q} \quad (4.50)$$

then we substitute Equation 4.39 into Equation 4.50 to yield the following:

$$\dot{\epsilon}^p = \left(\dot{\epsilon} - \frac{\dot{\mathbf{S}}}{2\mu} \right) : \mathbf{Q} \quad (4.51)$$

Finally, we will take Equation 4.51 and substitute it into Equation 4.35, take the differenced form by multiplying through by Δt , and solve for ϵ_t^p to give the following result:

$$\epsilon_t^p = \epsilon_{t-\Delta t}^p + \sqrt{\frac{2}{3}} \left(\Delta \mathbf{e}_{t-\Delta t/2} - \frac{\mathbf{S}_t - \mathbf{S}_{t-\Delta t}}{2\mu} \right) : \mathbf{Q}_{t-\Delta t/2} \quad (4.52)$$

where,

$$\mathbf{Q}_{t-\Delta t/2} = \frac{\mathbf{Q}_t + \mathbf{Q}_{t-\Delta t}}{2} \quad (4.53)$$

The current value of equivalent plastic strain, ϵ^p , can now be solved for by using Equation 4.52.

4.9 Constitutive Model

With the fundamental theory in hand, we will turn to the numerical implementation of the constitutive model. The viscoplastic constitutive law we adopted was used in Camacho and Ortiz [8] and modified by Warren and Tabbara [66] to ignore temperature effects resulting in the form shown in Equation 4.54

$$G = g \left(1 + \frac{\dot{\epsilon}^p}{\dot{\epsilon}_0^p} \right)^{1/m} \quad (4.54)$$

where $\dot{\epsilon}^p$ is the equivalent plastic strain rate, $\dot{\epsilon}_0^p$ is a reference equivalent plastic strain rate, m is the strain-rate exponent, and g defines the work hardening component of the model and is given by Equation 4.55

$$g = Y \left(1 + \frac{\epsilon^p}{\epsilon_0^p} \right)^{1/n} \quad (4.55)$$

where, Y is the quasi-static yield stress, ϵ^p is the equivalent plastic strain, ϵ_0^p is the reference equivalent plastic strain, and n is a strain hardening parameter. This model is phenomenological in nature with n , m , ϵ_0^p , and $\dot{\epsilon}_0^p$ being curve fit parameters determined from experimental data.

Momentarily returning to Equation 4.44, we show the relationship that we will use to numerically find $\Delta\lambda$. If we use the constitutive model of Equation 4.54 as the yield function,

Equation 4.44 becomes

$$\Delta e_{t-\Delta t/2} - \Delta \lambda_{t-\Delta t/2} - \frac{1}{2\mu} \left[\sqrt{\frac{2}{3}} Y \left(1 + \frac{\varepsilon_{t-\Delta t}^p}{\varepsilon_0^p} \right)^{1/n} \left(1 + \sqrt{\frac{2}{3}} \frac{\Delta \lambda_{t-\Delta t/2}}{\Delta t \dot{\varepsilon}_0^p} \right)^{1/m} - S_{t-\Delta t} \right] = 0 \quad (4.56)$$

And it follows that the yield surface G_t will be defined by:

$$G_t = Y \left(1 + \frac{\varepsilon_{t-\Delta t}^p}{\varepsilon_0^p} \right)^{1/n} \left(1 + \sqrt{\frac{2}{3}} \frac{\Delta \lambda_{t-\Delta t/2}}{\Delta t \dot{\varepsilon}_0^p} \right)^{1/m} \quad (4.57)$$

4.10 Numerical Simulations

The viscoplastic constitutive model presented in the previous section was implemented into the explicit peridynamics code Emu. In a typical finite element code, when a new model is introduced, it is customary to run a uniaxial stress test on a single element in order to verify that the constitutive response reproduces the experimental data. In the peridynamic framework, a single node simulation will not suffice because a minimum number of nodes is necessary to calculate a stress tensor. Instead, a model consisting of 3825 nodes representing a cylindrical tensile test specimen was simulated for comparison to experimental data. The simulation was run at an engineering strain rate of 8300/s. Boundary conditions are applied by giving a region of nodes on either ends of the bar a constant velocity. This could also be achieved by applying a prescribed displacement or body force density to a region of nodes. The material parameters used correspond to a data fit to 6061-T6 aluminum provided in Song et. al [62]. The experiments were conducted using pulse shaped Kolsky bar experiments to ensure a constant engineering strain rate of 8300/s. The constitutive parameters are as follows: $E = 68.9$ GPa, $\nu = 0.333$, $Y = 276$ MPa, $n = 13.5$, $m = 44.0$, $\varepsilon_0^p = 0.001$ /s, and $\dot{\varepsilon}_0^p = 1000$ /s. Figure 4.3 shows true stress as a function of Lagrangian strain for the simulations. The strain measurement from the simulation was calculated by using the Green-St. Venant formulation from the approximate deformation gradient as shown in Equation 4.58.

$$\mathbf{E} = \frac{1}{2} (\mathbf{F}^T \mathbf{F} - \mathbf{I}) \quad (4.58)$$

The numerical implementation of the constitutive model matches the experimental data very well. Currently, the constitutive model is only implemented in the explicit peridynamics code, Emu, which makes running the simulation at quasi-static rates nearly impossible due to conditions which require a very small time step; consequently, only a comparison at the high rate was done.

In order to validate⁵ the numerical implementation of the viscoplastic constitutive model into Emu, Taylor impact experimental results were simulated. A set of Taylor impact tests

⁵Additional validation was done on an elastic constitutive model, comparing simulations to analytics solutions. This work is included in Appendix G.

were conducted on 6061-T6 aluminum by Anderson et. al [2]. This data included normalized length and diameter measurements as well as a selection of Dynamic Structured Light (DSL) images of the deformed specimens. The test specimens were 3.175 cm long with a diameter of 6.35 mm ($L/D = 5$). The tests were conducted at impact speeds between 26 and 440 m/s; however, at an impact speed of 363 m/s and above, post test examination of the Taylor impact specimens showed significant “mushrooming” and failure at the impact end. While failure can be modeled with peridynamics and Emu it is beyond the scope of this validation exercise; therefore, these experiments were not attempted in numerical simulation. The Emu simulations were performed with a resolution of 40 nodes across the diameter of the specimen, resulting in 252,800 total nodes. The length scale parameter, δ , was chosen to be $3.05 \cdot \Delta x$ where Δx is the distance between adjacent material particles. Simulations were also ran at $\delta = 4 \cdot \Delta x$ and $\delta = 5 \cdot \Delta x$ to investigate the length scale effect. As expected because these simulations were intended to investigate bulk response (change in length/diameter), the change in δ had little to no effect on the simulation results. Figure 4.4 shows the normalized length (final length divided by initial length) for the Taylor impact experiments and the numerical simulations using the Emu code with our viscoplastic model. Figure 4.5 shows the normalized diameter at the impact face for the Taylor experiments and the numerical simulations. Both the length and diameter calculations match the experimental data well. For a qualitative comparison of deformation, one of the Emu simulations is shown next to the DSL Image from tests conducted at 289 m/s impact speed in Figure 4.6. Here again we see a good qualitative comparison of the deformation.

Figure 4.3: Comparison of experimental data with numerical simulation at nominal engineering strain rate of 8300/s.

Figure 4.4: Normalized length comparison.

Figure 4.5: Normalized diameter comparison.

Figure 4.6: Qualitative comparison of post test deformation from DSL image with numerical simulation at 289 m/s impact speed.

These simulations suggest the viability of using peridynamics to model materials that exhibit viscoplasticity with hardening.

4.11 Concluding Remarks

In this chapter, an elastic, viscoplastic constitutive relationship is implemented into a peridynamic numerical analysis code with the use of force-vector states. The model is phenomenological and uses parameters fit to experimental data. The model was fit to high strain-rate constitutive data taken from Kolsky bar experiments on 6061-T6 aluminum. The model is then used to reproduce experimental results from Taylor impact tests of aluminum. The normalized length and diameter results from the calculations match the experimental results very well, and qualitative comparisons of post test deformation also compare well. This chapter demonstrates the ability to utilize conventional constitutive models within the state-based peridynamic framework. More importantly, this model will be extremely useful in our modeling of the inelastic and failure response of our 4340 steel samples as described in the next chapter.

5 Fracture Model and Numerical Simulation

5.1 Introduction

In Chapter 3, experiments were reported that showed a rate dependence of the dynamic crack initiation of a 4340 steel. An engineering analyst would use the knowledge of this rate dependence in order to predict material failure in structures that have high-rate deformations such as blast and impact. The first step to model these scenarios is to have a rate dependent constitutive model; a method for implementing such a model into a peridynamic explicit dynamics code was described in Chapter 4. The next step is to implement a failure criterion into the peridynamic framework that can use the knowledge of the rate dependent crack initiation toughness as an input to the model. A novel failure criterion and explanation of its implementation along with validation simulations is presented in this chapter.

5.2 Failure Model

The method of damage (failure, cracks, etc.) nucleation, coalescence, and propagation within the peridynamic model is through the permanent breaking of “bonds”. The word “bond” is used loosely in this context only to describe the relationship between two material points and can be thought of abstractly as an interaction potential; there is not necessarily a notion of direct connectivity such as a spring-like force. This is especially the case within the state-based peridynamic framework where the state-forces could potentially act in any conceivable direction, not just colinear with the position vector, and certainly not in an equal-and-opposite fashion such is the case in bond-based peridynamics. Figure 5.1 shows a notional illustration of this relationship where, following the notation from Chapter 1, ξ represents the “bond” and the $\underline{\mathbf{T}}$ ’s are the force-vector states.

In the numerical simulation of fracture many methods have been utilized to characterize when a material might fail. A few examples are the plastic strain to failure, stress triaxiality, lode angle dependence, etc. Most of these methods have some dependence on either the stress or strain histories. Since peridynamics is cast in a form that does not require the notion

Figure 5.1: Illustration of relationship between state-forces and “bond.”

of stress (although we used stress as a convenience for material modeling in Chapter 4), we wish to develop a failure criterion derived not from any stress or strain criterion, but instead using thermodynamic notions of work or energy. We can calculate the amount of energy density stored a bond¹, w_{ξ} , by projecting the force vector-states onto the relative displacement vector. The calculation is performed by Equation 5.1.

$$w_{\xi} = \int_0^{\eta(t_{final})} \{ \underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}', t] \langle \mathbf{x} - \mathbf{x}' \rangle \} \cdot d\boldsymbol{\eta} \quad (5.1)$$

where the integrand of Equation 5.1 is known as the *dual force density*. Recall from Chapter 4 that the relative displacement vector $\boldsymbol{\eta}$ is defined by Equation 5.2

$$\boldsymbol{\eta} = \mathbf{u}[\mathbf{x}', t] - \mathbf{u}[\mathbf{x}, t] \quad (5.2)$$

A schematic of the bond kinematics is shown in Figure 5.2. Equation 5.1 defines w_{ξ} as having units of energy per unit volume squared. It represents an amount of work density done on a bond due to displacing the two material points $\mathbf{x}$ and $\mathbf{x}'$ relative to one another from zero to some final scalar value of displacement, $\eta(t_{final})$, which is a function of time. This projection neglects any work done on the points due to rigid body translation. The motivation for this idea comes from the well known physics equation where the work done to a body is the force acting on it, $\mathbf{f}$, integrated over the path length, $\mathbf{s}$, as shown in Equation 5.3

$$W = \int \mathbf{f} \cdot d\mathbf{s} \quad (5.3)$$

However, in this case the work is actually an energy density, the force is the dual force density, and the path is the relative displacement.

Although, the formal proof is not attempted here, it is hypothesized that by integrating w_{ξ} over the entire volume of the non-local horizon, $\mathcal{H}$, of radius δ , we could expect the

¹We will drop the quotation marks from the word bond henceforth, but we maintain the same notion of interaction as described in the first paragraph of Section 5.2

Figure 5.2: Schematic of bond kinematics.

result to converge in the limit as $\delta \rightarrow 0$ to the classic notion of strain energy density, w , as illustrated in Equation 5.4.

$$w = \int \boldsymbol{\sigma} : d\boldsymbol{\varepsilon} = \lim_{\delta \rightarrow 0} \int_{\mathcal{H}} w_{\boldsymbol{\xi}} dV_{\boldsymbol{\xi}} \quad (5.4)$$

Of course, we would expect this to be true only if we assume a smooth deformation for the existence of the partial derivatives contained in the strain tensor, $\boldsymbol{\varepsilon}$.

Figure 5.3 shows an example of how a viscoplastic material could potentially reach the same bond energy density with different levels of relative displacement at t_{final} . The values of η and $\underline{t}$'s represent some scalar projection of the vector values shown in Equation 5.1, possibly the projection of the vectors onto the axial direction in a standard tensile test experiment. In this idealized example, $w_{\xi_1} = w_{\xi_2}$ even though the relative displacements, η_1 and η_2 , have different ultimate values. This is because the material behaves differently (e.g., exhibits rate dependence) when displaced at the two different rates, $\dot{\eta}_1$ and $\dot{\eta}_2$.

We will assume that the energy density contained in a bond is fully recoverable² by reversing the deformation, unless it exceeds some critical energy density, w_c . Let us attempt to define w_c in terms of material property that can be experimentally determined. Referring to Figure 5.4, let us consider all points A along the dashed line, $0 < z < \delta$, connected to all points B across a fracture plane of unit area and within a spherical cap of radius δ with respect to A (the shaded area in Figure 5.4). If we assume there is a critical energy density, w_c , associated with moving each point A relative to each point B , that when exceeded will cause the removal of any potential between the two points (irreversible bond breakage), then we can sum up all of these energy densities through integration and equate the result with

²The bond energy density will only be fully recoverable if we assume a classically hyperelastic material model, if we assume a dissipative material model then some of the work done on the bond may be permanent.

Figure 5.3: Example of equivalent w_ξ and different $\eta(t_{final})$ for two relative displacement rates.

the energy release rate, G_f . That is, the energy required to open a new fracture surface of unit area. This equation is as follows:

$$G_f = \int_0^\delta \int_0^{2\pi} \int_z^\delta \int_0^{\cos^{-1} z/\xi} w_c \xi^2 \sin \phi d\phi d\xi d\theta dz \quad (5.5)$$

When evaluated and solved for w_c , Equation 5.5 reduces to:

$$w_c = \frac{4G_f}{\pi\delta^4} \quad (5.6)$$

Now we have a critical value of energy density that is based solely on material properties (recall that δ is considered a material property). We can compare this critical energy density to the individual bond energy densities calculated via Equation 5.1 to determine when the bonds will individually fail. Cracks will nucleate and grow when a number of bond failures coalesce into a surface and propagate. This phenomenon will emerge naturally without the need to specify when and where the cracks will appear through some external criterion. Another advantage to the peridynamic model and allowing the bonds to break in this fashion is that it leads to an unambiguous notion of damage. The percentage of material damage a continuum point has undergone is simply the percentage of broken bonds. For example, if one material point interacts with one hundred others and one bond is broken, the material point is considered 1% damaged.

To numerically implement this failure criterion with the constitutive model described in Chapter 4, we will activate bond breakage through the use of the influence function contained

Figure 5.4: Schematic of fracture surface.

in the deformation gradient and shape tensors. Recall the formula for approximating the deformation gradient from Chapter 4 reproduced here as Equation 5.7.

$$\mathbf{F}[\mathbf{x}, t] = \left[\int_{\mathcal{H}} \omega(|\boldsymbol{\xi}|) (\mathbf{Y} \langle \boldsymbol{\xi} \rangle \otimes \boldsymbol{\xi}) dV_{\mathbf{x}'} \right] \mathbf{K}^{-1} \quad (5.7)$$

The term $\omega(|\boldsymbol{\xi}|)$ was defined as an influence function. It can be used to assign a weight to the amount of influence each bond within the horizon exerts on the point $\mathbf{x}$. We can use it to implement damage by setting the influence to zero for the bonds that are broken. Therefore, the failure criterion expressed mathematically is as follows:

$$\omega(|\boldsymbol{\xi}|) = \begin{cases} 0 & w_{\boldsymbol{\xi}} > w_c \\ 1 & \text{otherwise} \end{cases} \quad (5.8)$$

When numerically implemented into the explicit dynamics code Emu, we calculate $w_{\boldsymbol{\xi}}$ for every bond at each time step in the simulation and compare it to w_c . If $w_{\boldsymbol{\xi}}$ exceeds w_c , then the influence function is set to zero for that bond, and the bond is effectively left out of the calculation of the deformation gradient at the next time step. The force that was exerted on the point $\mathbf{x}$ by the broken bond will now have to be assumed by the remaining intact bonds. This additional load on the intact bonds may cause them to subsequently break thereby mimicing damage propagation throughout the structure.

Figure 5.5: Comparison of data to simulation at strain rates of 1150/s and 2900/s.

5.3 Numerical Simulations

The failure criterion described in Section 5.2 was implemented into the peridynamic computational mechanics code Emu and a selection of experiments from Chapter 3 were simulated. Because the samples consisted of 4340 steel, the constitutive response for this material needed to be validated. The constitutive model described in Chapter 4 was fit to experimental data for 4340 with a similar heat treatment and Rockwell hardness published by Frew et al. [20]. The fitted constitutive parameters for the 4340 steel are $E = 210$ GPa, $\nu = 0.29$, $Y = 1116$ MPa, $n = 65$, $m = 27.5$, $\varepsilon_0^p = 5.417 \times 10^{-3}$ m/m, and $\dot{\varepsilon}_0^p = 5.940 \times 10^{-3}$ /s. The model fit is demonstrated along with reported data at two different strain rates in Figure 5.5.

The experiments reported in Chapter 3 were done to detect the dynamic crack initiation toughness of the 4340 steel samples. In order to use K_{Ic} as an input to this failure model, we have to resort to the relationship from plane strain linear elastic fracture mechanics shown in Equation 5.9

$$G_f = \frac{K_{Ic}^2}{E} (1 - \nu^2) \quad (5.9)$$

where, E is the elastic (Young's) modulus and ν is Poisson's Ratio, which results in the failure criterion based on K_{Ic} shown in Equation 5.10.

$$w_c = \frac{4K_{Ic}^2}{\pi E \delta^4} (1 - \nu^2) \quad (5.10)$$

Now someone may pose the question, “Why are we resorting to linear elastic fracture mechanics (LEFM) when the peridynamic theory does not exhibit a crack tip stress singularity (recall that the singular stress field in the classical theory is the reason one uses K_{Ic})?” The answer to this question has to do with our shortcomings as experimentalists, not from the peridynamic theory or the failure model. We use K_{Ic} here as a convenience because it is the easiest of the crack tip physics variables to measure. If we possessed measurements of G or the J -Integral directly (which would not limit us to LEFM) we could use them as inputs to the failure model and proceed with modeling any failure (e.g., elastic-plastic) in a straightforward fashion.

The boundary conditions we applied in the simulations come from the boundary velocity measurements in the Kolsky experiments. The measured velocities are applied as initial conditions to a four point bend beam that has been discretized into peridynamic nodes. Figure 5.6 shows the boundary regions where the velocities were applied. Notice that only a single row of nodes was segmented out and made into boundary regions. This was done as not to impart any moments in the region where the boundary conditions were applied. Also, note that the velocity vectors all point in the same direction; therefore moving the entire sample to the left during the simulation. The deformation comes from the v_1 velocities being much higher in magnitude than the v_2 velocities. This is shown to be obvious by reexamining the sample boundary velocities reported in Chapter 3 shown here in Figure 5.7. The boundary condition applied to boundary region 5 shown in Figure 5.6 was a condition applied to the entire body that restricts displacements in the direction normal to the plane of the sample. This was done in order to mimic plane strain conditions without the need to actually model a very thick sample. The resulting sample has 5 nodes in the thickness direction, 50 nodes across the sample width, and 214 nodes along the sample length, resulting in 53 500 total nodes.

For test number T36 shown in Figure 5.7, the time-to-fracture was approximately 27 μ s. The measure of comparison for the simulation is the time-to-fracture, therefore, the simulation was only run out to around 50 μ s. After this time, the boundary conditions become less realistic since the sample begins to slide along the supports after crack initiation and this motion is not modeled in the simulation. Any comparisons to crack propagation can only be qualitative because of the simplified boundary condition not imposed in the simulations which does not represent the experiment exactly. Furthermore, no robust experimental measurements were made on the propagation speed.

Because the peridynamic model allows for arbitrary crack growth through the accumulation of broken bonds without specifying when or where the cracks will nucleate and grow, it can be difficult to quantitatively track crack propagation in complex structures. However, because the sample modeled here is fairly simple and it is known from experimental observations where the crack will initiate, a simple algorithm was written to detect when roughly 50% of the bonds are broken thereby representing a crack.³ A selection of the experiments

³The 50% damage criterion comes from the fact that for a node to be on the surface of a crack roughly half of the bonds across the failure plane will be irreversibly broken, and roughly half the bonds will still be connected to the interior of the body

(a) Boundary regions.

(b) Boundary region 2 zoom.

Figure 5.6: Boundary regions.

Figure 5.7: Sample boundary velocities from test T36.

were modeled, resulting in good agreement with the times-to-fracture for each experiment. Results from two different simulated loading rates are compared to the experimental crack initiation times-to-fracture in Figure 5.8. The vertical dashed line in the figures represents the experimentally measured times-to-fracture. The solid line represents the tracking of the crack tip position in the simulations. Because the coordinate system origin (shown in Figure 5.6) is on the right hand boundary of the sample, the maximum of the ordinate axes in the figures represents the place where the crack would break the sample in half. The initial value of the crack tip position represents the initial length of the crack taken from the experimental measurements. Figure 5.8a uses the value of $K_{Ic} = 65 \text{ MPa}\sqrt{\text{m}}$ as an input to the failure model at a loading rate of $\dot{K}_I = 2.407 \times 10^6 \text{ MPa}\sqrt{\text{m}}/\text{s}$ which is labeled as Loading Rate 1 in the figure. Figure 5.8b uses the value of $K_{Ic} = 139 \text{ MPa}\sqrt{\text{m}}$ as an input to the failure model at a loading rate of $\dot{K}_I = 4.343 \times 10^6 \text{ MPa}\sqrt{\text{m}}/\text{s}$ labeled as Loading Rate 2 in the figure. Both simulations show very good comparisons to the experimental time-to-fractures.

In order to visualize the overall deformation, crack initiation, and propagation a set of images from the simulations were sampled and sequenced in Appendix E. Figure 5.9 shows an animation⁴ of the simulation.

As mentioned in Chapter 3 a subset of experiments were conducted at Purdue University

⁴If the reader is viewing the electronic PDF of this document in Adobe Acrobat[®] 9 or newer with JavaScript enabled, click on Figure 5.9 to view the animation; otherwise, refer to Appendix E to view the sequenced images.

(a) Test T36 (Loading rate 1).

(b) Test T20 (Loading rate 2).

Figure 5.8: Comparison of time-to-fracture from experiment and simulation.

Figure 5.9: Simulation results showing crack initiation and propagation.

and a Cordin high-speed rotating mirror camera was used to capture the crack initiation and propagation. These samples were 4340 steel, but had a slightly different heat treatment than the samples reported in Figure 3.14; therefore, the dynamic crack initiation toughness measurements were not reported with the others. One sample from this group was simulated using Emu; images from the simulation were sampled at the same frame rate as the camera ($\approx 4 \mu\text{s}$) data and comparisons were made. The sampled results are shown in Appendix E and the resulting simulation is shown in Figure 5.10.

The simulations shows good quantitative correlation with the crack initiation time. By comparing the visual results from the simulation and the camera footage we see that the propagation speed as well qualitatively compares as well. This is somewhat surprising being that the failure model uses only K_{Ic} as an input. This phenomenon should be researched further in future work and compared to quantitative crack speed data.

5.4 Concluding Remarks

This chapter motivated and presented a novel energy based failure criterion that was implemented into a peridynamics continuum mechanics code and compared to experimental results. By using experimental crack initiation toughness measurements and the experimental boundary conditions as inputs to the code, the failure model was able to reproduce time-to-fracture measurements as well as suggestively reproduce crack propagation speed.

One aspect of the model that needs to be further researched is the fact that the critical energy density, w_c , is identical whether the bond is in tension or compression. For some engineering materials, such as concrete, this may not be a realistic approximation; however, a different derivation for w_c , which would include differences for tension or compression, could be easily incorporated. Overall the model seems to perform well for the limited number of experiments simulated and allows us to account for unguided crack propagation within a consistent mathematical framework.

The simulations presented in this chapter use the recorded values of K_{Ic} as individual inputs at each loading rate, meaning the analyst must have some a priori knowledge of the loading rate of the experiment in order to chose the appropriate value of K_{Ic} . However, it would be very simple to implement a model where K_{Ic} is a curve instead of a single value and the simulations could approximate the near crack tip value of $\dot{K}_I$ and use the value of K_{Ic} accordingly.

Figure 5.10: Comparison of simulation to experimental camera data.

6 Summary and Recommendations

The work in this dissertation had two distinctly different areas of original research. Chapter 3, Chapter 4, and Chapter 5 each had sections at the end which contained some concluding remarks on the major contributions in each area. The most important original contributions are highlighted below:

- Experiments
 - A novel experimental and data reduction technique was used to record dynamic crack initiation toughness measurements of a 4340 steel utilizing the Kolsky apparatus.
 - Data was presented for 4340 steel at two different nominal loading rates of which are shown to be very near constant by using pulse shaping techniques to shape the loading pulse.
 - The 4340 steel samples were shown to have a rate dependence for the dynamic crack initiation toughness.
- Peridynamic Simulation
 - The research presented in Chapter 4 was the first implementation of a (state-based) viscoplastic constitutive model into the peridynamic framework.
 - The constitutive model validation was the first peridynamic implementation to quantitatively compare to experimental results and showed excellent agreement to the Taylor anvil impact data.
 - A novel failure model using an energy based criterion was hypothesized and implemented into a peridynamics numerical code.
 - The failure model was validated on a significant class of problems, (i.e., mode I dynamic fracture) by simulating the experimental results recorded in Chapter 3 using the dynamic crack initiation toughness as inputs to the model.

The concluding remarks of Chapter 3 give several ideas for future enhancements of the experimental technique. Most notably, if the sample size were adjusted or the Kolsky bar diameter increased, one could incorporate the impact and support tups into the end of the

bars to eliminate the need for special timing corrections to account for the wave propagation that takes place in the gage section.

For the peridynamic modeling, there is a lifetime of research to be undertaken in this new field of continuum mechanics. A few straightforward additions to the research presented here would be to investigate convergence and mesh sensitivity of the failure and constitutive models. The next step would be to investigate failure in complex structures where the crack initiation and propagation directions may be unknown a priori. If the structure exhibits fragmentation, comparisons of fragment size distribution¹ could be undertaken. The research presented in the dissertation should also make contributions to the science of penetration mechanics. There are still many unsolved phenomena in plate perforations such as the different types of failure (e.g., cavity expansion, spall, plugging). A few simple simulations of the perforation of an aluminum plate, where the plate is modeled with the constitutive model of Chapter 4 and the failure model of Chapter 5 are shown in Figure 6.1. The simulations were run with a two rigid projectiles, one with an ogive nose, and one with a flat cylindrical nose. Both projectiles had the same initial velocity and angle-of-incidence to the plate. Notice the different failure patterns the different nose shapes impart on the plate. Perforation with the ogive nose gives rise to the mechanism of a cavity expansion whereas the cylindrical nose is stopped in the plate. But one can see the beginnings of a plug being pushed through the plate. These simulations were run with a very course mesh and were not intended to simulate any particular experiment, they are just used to notionally show other applications and areas of research for the modeling of materials and material failure with peridynamics.

The future direction of this author's research will include looking at peridynamic mesh sensitivity convergence of crack initiation and propagation as well as failure pattern convergence when the mesh node locations are randomly perturbed in the reference configuration (a method of introducing material heterogeneity). More complex fracture experiments (i.e., multiple cracks) will be simulated as well penetration and perforation comparisons to experimental data. Future interests also include implementing constitutive and failure models for concrete, in a similar fashion as those described in this work, and studying damage initiation and propagation in that complex but important engineering material.

¹Preliminary work in this area has already been undertaken by Dr. Stewart A. Silling using the constitutive model presented in Chapter 4. Some simulations showing good correlation to experimental data were shown by Dr. David J. Littlewood at a presentation at US National Congress on Computational Mechanics 10 in Columbus, Ohio, July 2009.

(a) Ogive Nose

(b) Flat Nose

Figure 6.1: Ogive and flat nose penetration of aluminum plate.

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A Loading Rate 1

(a) Raw data.

(b) Incident signal.

(c) Transmitted signal.

(d) Force equilibrium.

(e) Sample boundary velocity.

(f) Stress intensity factor.

Figure A.1: Sample T08.

(a) Raw data.

(b) Incident signal.

(c) Transmitted signal.

(d) Force equilibrium.

(e) Sample boundary velocity.

(f) Stress intensity factor.

Figure A.2: Sample T12.

(a) Raw data.

(b) Incident signal.

(c) Transmitted signal.

(d) Force equilibrium.

(e) Sample boundary velocity.

(f) Stress intensity factor.

Figure A.3: Sample T27.

(a) Raw data.

(b) Incident signal.

(c) Transmitted signal.

(d) Force equilibrium.

(e) Sample boundary velocity.

(f) Stress intensity factor.

Figure A.4: Sample T36.

B Loading Rate 2

(a) Raw data.

(b) Incident signal.

(c) Transmitted signal.

(d) Force equilibrium.

(e) Sample boundary velocity.

(f) Stress intensity factor.

Figure B.1: Sample T19.

(a) Raw data.

(b) Incident signal.

(c) Transmitted signal.

(d) Force equilibrium.

(e) Sample boundary velocity.

(f) Stress intensity factor.

Figure B.2: Sample T20.

(a) Raw data.

(b) Incident signal.

(c) Transmitted signal.

(d) Force equilibrium.

(e) Sample boundary velocity.

(f) Stress intensity factor.

Figure B.3: Sample T21.

(a) Raw data.

(b) Incident signal.

(c) Transmitted signal.

(d) Force equilibrium.

(e) Sample boundary velocity.

(f) Stress intensity factor.

Figure B.4: Sample T23.

(a) Raw data.

(b) Incident signal.

(c) Transmitted signal.

(d) Force equilibrium.

(e) Sample boundary velocity.

(f) Stress intensity factor.

Figure B.5: Sample T32.

C Machine Drawings

Figure C.2: Machine drawing of incident tup bracket.

Figure C.3: Machine drawing of transmitter support bracket.

D Sample Dimensions

Table D.1: Sample dimensions in millimeters.

Sample No.	W	B	a_1	a_2	a_3	a
T08	7.553	14.118	7.635	7.656	7.479	7.590
T12	7.581	14.436	7.237	7.163	7.334	7.245
T27	7.606	14.567	7.317	7.300	7.478	7.365
T36	7.649	14.064	7.165	7.528	7.568	7.420
T19	7.726	14.020	6.948	7.195	7.232	7.125
T20	7.485	13.940	6.573	6.594	6.506	6.557
T21	7.504	14.133	7.266	7.359	7.183	7.269
T23	7.627	14.399	7.135	7.255	7.086	7.158
T32	7.620	13.984	6.970	7.173	7.176	7.106

E Sequenced Images of Crack Initiation and Propagation in Beam

Figure E.1: Simulation of test T36.

Figure E.1: Simulation of test T36 (cont.).

Figure E.1: Simulation of test T36 (cont.).

Figure E.1: Simulation of test T36 (cont.).

(i) $t \approx 0 \mu\text{s}$

(ii) $t \approx 2 \mu\text{s}$

(iii) $t \approx 4 \mu\text{s}$

(iv) $t \approx 6 \mu\text{s}$

Figure E.2: Comparison of simulation to experiment.

(v) $t \approx 8 \mu\text{s}$

(vi) $t \approx 10 \mu\text{s}$

(vii) $t \approx 12 \mu\text{s}$

(viii) $t \approx 14 \mu\text{s}$

Figure E.2: Comparison of simulation to experiment (cont.).

(ix) $t \approx 16 \mu\text{s}$

(x) $t \approx 18 \mu\text{s}$

(xi) $t \approx 20 \mu\text{s}$

(xii) $t \approx 22 \mu\text{s}$

Figure E.2: Comparison of simulation to experiment (cont.).

(xiii) $t \approx 24 \mu\text{s}$

(xiv) $t \approx 26 \mu\text{s}$

(xv) $t \approx 28 \mu\text{s}$

(xvi) $t \approx 30 \mu\text{s}$

Figure E.2: Comparison of simulation to experiment (cont.).

(xvii) $t \approx 32 \mu\text{s}$

(xviii) $t \approx 34 \mu\text{s}$

(xix) $t \approx 36 \mu\text{s}$

(xx) $t \approx 38 \mu\text{s}$

Figure E.2: Comparison of simulation to experiment (cont.).

(xxi) $t \approx 40 \mu\text{s}$

(xxii) $t \approx 42 \mu\text{s}$

(xxiii) $t \approx 44 \mu\text{s}$

(xxiv) $t \approx 46 \mu\text{s}$

Figure E.2: Comparison of simulation to experiment (cont.).

(xxv) $t \approx 48 \mu\text{s}$

(xxvi) $t \approx 50 \mu\text{s}$

(xxvii) $t \approx 52 \mu\text{s}$

(xxviii) $t \approx 54 \mu\text{s}$

Figure E.2: Comparison of simulation to experiment (cont.).

(xxix) $t \approx 56 \mu\text{s}$

(xxx) $t \approx 58 \mu\text{s}$

(xxxi) $t \approx 60 \mu\text{s}$

(xxxii) $t \approx 62 \mu\text{s}$

Figure E.2: Comparison of simulation to experiment (cont.).

F Additional Derivations of Peridynamic Notions

F.1 Definitions

Before we begin the derivation of the peridynamic equation of motion let us define a few properties that will prove useful. All definitions from the body of the dissertation hold unless redefined here.

F.1.1 Vector-State Point Product

The *point product* of two states $\underline{\mathbf{A}} \in \mathcal{A}_{m+p}$ and $\underline{\mathbf{B}} \in \mathcal{A}_p$ is a state in $\mathcal{A}_m$ defined by:

$$(\underline{\mathbf{A}} \cdot \underline{\mathbf{B}})_{i_1 \dots i_m} \langle \xi \rangle = \underline{A}_{i_1 \dots i_m j_1 \dots j_p} \langle \xi \rangle \underline{B}_{j_1 \dots j_p} \langle \xi \rangle \quad \forall \xi \in \mathcal{H} \quad (\text{F.1})$$

and similarly,

$$(\underline{\mathbf{B}} \cdot \underline{\mathbf{A}})_{i_1 \dots i_m} \langle \xi \rangle = \underline{B}_{j_1 \dots j_p} \langle \xi \rangle \underline{A}_{j_1 \dots j_p i_1 \dots i_m} \langle \xi \rangle \quad \forall \xi \in \mathcal{H} \quad (\text{F.2})$$

If the two states are of the same order then $\underline{\mathbf{A}} \cdot \underline{\mathbf{B}} = \underline{\mathbf{B}} \cdot \underline{\mathbf{A}}$.

F.1.2 Vector-State Dot Product

The *dot product* of two states $\underline{\mathbf{A}}$ and $\underline{\mathbf{B}}$ is defined by:

$$\underline{\mathbf{A}} \bullet \underline{\mathbf{B}} = \int_{\mathcal{H}} (\underline{\mathbf{A}} \cdot \underline{\mathbf{B}}) \langle \xi \rangle dV_{\xi} \quad (\text{F.3})$$

Note that, once again, if the two states are of the same order then $\underline{\mathbf{A}} \bullet \underline{\mathbf{B}} = \underline{\mathbf{B}} \bullet \underline{\mathbf{A}}$.

F.1.3 Fréchet Derivative

Let Ψ be a function of a state $\Psi(\cdot) : \mathcal{A}_m \rightarrow \mathcal{L}_n$, where $\mathcal{L}_n$ is the set of all tensors of order n . Suppose there exists a state-valued function denoted $\nabla \Psi \in \mathcal{A}_{m+n}$ such that for any $\underline{\mathbf{A}} \in \mathcal{A}_m$

an any $\Delta \underline{\mathbf{A}} \in \mathcal{A}_m$,

$$\Psi(\underline{\mathbf{A}} + \Delta \underline{\mathbf{A}}) = \Psi(\underline{\mathbf{A}}) + \nabla \Psi(\underline{\mathbf{A}}) \bullet \Delta \underline{\mathbf{A}} + \mathcal{O}(|\Delta \underline{\mathbf{A}}|) \quad (\text{F.4})$$

where $\mathcal{O}(|\Delta \underline{\mathbf{A}}|)$ represents higher order terms of $\Delta \underline{\mathbf{A}}$, then Ψ is said to be *differentiable* and $\nabla \Psi$ is called the *Fréchet derivative* of Ψ .

F.1.3.1 Example

Let $\Psi(\underline{\mathbf{A}}) = 2\underline{\mathbf{A}} \bullet \underline{\mathbf{A}} \quad \forall \underline{\mathbf{A}} \in \mathcal{V}$

$$\begin{aligned} \Psi(\underline{\mathbf{A}} + \Delta \underline{\mathbf{A}}) &= 2(\underline{\mathbf{A}} + \Delta \underline{\mathbf{A}}) \bullet (\underline{\mathbf{A}} + \Delta \underline{\mathbf{A}}) \\ &= 2\underline{\mathbf{A}} \bullet \underline{\mathbf{A}} + 4\underline{\mathbf{A}} \bullet \Delta \underline{\mathbf{A}} + \mathcal{O}(|\Delta \underline{\mathbf{A}}|) \end{aligned}$$

hence $\nabla \Psi(\underline{\mathbf{A}}) = 4\underline{\mathbf{A}}$.

F.2 Derivation of Peridynamic Equation of Motion

In order to derive the peridynamic equation of motion let us consider a closed, bounded peridynamic body $\mathcal{B}$, similar to that shown in Figure 1.3a, with strain energy density given by $\hat{W}(\underline{\mathbf{Y}}[\mathbf{x}, t])$ where $\underline{\mathbf{Y}}[\mathbf{x}, t]$ is the deformation state shown in Equation F.5,

$$\begin{aligned} \underline{\mathbf{Y}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle &= (\mathbf{u}[\mathbf{x}', t] + \mathbf{x}') - (\mathbf{u}[\mathbf{x}, t] + \mathbf{x}) \\ &= \mathbf{y}[\mathbf{x}', t] - \mathbf{y}[\mathbf{x}, t] \end{aligned} \quad (\text{F.5})$$

for all points $\mathbf{x}, \mathbf{x}' \in \mathcal{B}$, where $\mathbf{u}$ is the displacement and $\mathbf{y}$ is the deformation. Let $\mathbf{b}$ be the prescribed body force density field. The total potential energy functional for any deformation is then as follows:

$$\Phi_{\mathbf{y}} = \int_{\mathcal{B}} \left(\hat{W}(\underline{\mathbf{Y}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle) - \mathbf{b}[\mathbf{x}, t] \cdot \mathbf{y}[\mathbf{x}, t] \right) dV_{\mathbf{x}} \quad (\text{F.6})$$

Let $\nabla \hat{W}$ denote the Fréchet derivative of $\hat{W}$, and define the peridynamic force-vector state as follows:

$$\underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle = \nabla \hat{W}(\underline{\mathbf{Y}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle) \quad (\text{F.7})$$

By properties of the Fréchet derivative, for any variation of the deformation $\delta \mathbf{y}$, we have the following:

$$\delta \hat{W}(\underline{\mathbf{Y}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle) = \underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle \bullet \delta \underline{\mathbf{Y}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle \quad (\text{F.8})$$

Substituting Equation F.8 into Equation F.5 and using the definition of a vector-state dot product we get the result shown in Equation F.9

$$\delta \hat{W}(\underline{\mathbf{Y}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle) = \int_{\mathcal{B}} \underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle \cdot (\delta \mathbf{y}[\mathbf{x}', t] - \delta \mathbf{y}[\mathbf{x}, t]) dV_{\mathbf{x}'} \quad (\text{F.9})$$

Now take the first variation of $\Phi_{\mathbf{y}}$ to get the following:

$$\delta\Phi_{\mathbf{y}} = \int_{\mathcal{B}} \left(\delta\hat{W}(\underline{\mathbf{Y}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle) - \mathbf{b}[\mathbf{x}, t] \cdot \delta\mathbf{y}[\mathbf{x}, t] \right) dV_{\mathbf{x}} \quad (\text{F.10})$$

Substituting Equation F.9 into Equation F.10 we have:

$$\delta\Phi_{\mathbf{y}} = \int_{\mathcal{B}} \left(\int_{\mathcal{B}} (\underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle \cdot (\delta\mathbf{y}[\mathbf{x}', t] - \delta\mathbf{y}[\mathbf{x}, t])) dV_{\mathbf{x}'} - \mathbf{b}[\mathbf{x}, t] \cdot \delta\mathbf{y}[\mathbf{x}, t] \right) dV_{\mathbf{x}} \quad (\text{F.11})$$

a change of variables $\mathbf{x}' \leftrightarrow \mathbf{x}$ yields:

$$\delta\Phi_{\mathbf{y}} = \int_{\mathcal{B}} \left(\int_{\mathcal{B}} (\underline{\mathbf{T}}[\mathbf{x}', t] \langle \mathbf{x} - \mathbf{x}' \rangle - \underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle) \cdot \delta\mathbf{y}[\mathbf{x}, t] dV_{\mathbf{x}'} - \mathbf{b}[\mathbf{x}, t] \cdot \delta\mathbf{y}[\mathbf{x}, t] \right) dV_{\mathbf{x}} \quad (\text{F.12})$$

or,

$$\delta\Phi_{\mathbf{y}} = \int_{\mathcal{B}} \left(\int_{\mathcal{B}} (\underline{\mathbf{T}}[\mathbf{x}', t] \langle \mathbf{x} - \mathbf{x}' \rangle - \underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle) dV_{\mathbf{x}'} - \mathbf{b}[\mathbf{x}, t] \right) \cdot \delta\mathbf{y}[\mathbf{x}, t] dV_{\mathbf{x}} \quad (\text{F.13})$$

For a deformation in which $\Phi_{\mathbf{y}}$ is stationary by definition, $\delta\Phi_{\mathbf{y}} = 0$, using this and assuming an arbitrary $\delta\mathbf{y}$ we get the peridynamic equilibrium equation shown in Equation F.14.

$$\int_{\mathcal{B}} (\underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}', t] \langle \mathbf{x} - \mathbf{x}' \rangle) dV_{\mathbf{x}'} + \mathbf{b}[\mathbf{x}, t] = 0 \quad (\text{F.14})$$

Using d'Alembert's principle, replacing $\mathbf{b}[\mathbf{x}, t]$ with $\mathbf{b}[\mathbf{x}, t] - \rho\ddot{\mathbf{y}}[\mathbf{x}, t]$ results in the peridynamic equation of motion,

$$\rho\ddot{\mathbf{y}}[\mathbf{x}, t] = \int_{\mathcal{B}} (\underline{\mathbf{T}}[\mathbf{x}, t] \langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}', t] \langle \mathbf{x} - \mathbf{x}' \rangle) dV_{\mathbf{x}'} + \mathbf{b}[\mathbf{x}, t] \quad (\text{F.15})$$

F.3 Conversion of Stress Tensor to Force-Vector States Derivation

Let us consider a hyperelastic material (in the sense of classical elasticity theory) with strain energy density, $\Omega(\mathbf{F})$, which is a function of the deformation gradient, $\mathbf{F}$. We wish to equate $\Omega(\mathbf{F})$ with peridynamic strain energy density, $\hat{W}(\underline{\mathbf{Y}}[\mathbf{x}, t])$ presented in Section F.2, i.e.,

$$\hat{W}(\underline{\mathbf{Y}}[\mathbf{x}, t]) = \Omega(\mathbf{F}[\mathbf{x}, t]) \quad (\text{F.16})$$

Recall Equation 4.8 from Section 4.2 reproduced here as Equation F.17 which approximates the deformation gradient from the deformation state.

$$\mathbf{F}[\mathbf{x}, t] = \left[\int_{\mathcal{H}} \omega\langle \boldsymbol{\xi} \rangle (\underline{\mathbf{Y}}\langle \boldsymbol{\xi} \rangle \otimes \boldsymbol{\xi}) dV_{\mathbf{x}'} \right] \mathbf{K}^{-1} \quad (\text{F.17})$$

We can use Equation F.17 to evaluate the Fréchet derivative by considering an incremental change in $\underline{\mathbf{Y}}$,

$$\begin{aligned}
\mathbf{F}(\underline{\mathbf{Y}} + \Delta \underline{\mathbf{Y}}) &= \int_{\mathcal{H}} \omega \langle \boldsymbol{\xi} \rangle (\underline{Y}_i \langle \boldsymbol{\xi} \rangle + \Delta \underline{Y}_i \langle \boldsymbol{\xi} \rangle) \xi_p K_{pj}^{-1} dV_{\boldsymbol{\xi}} \\
&= \mathbf{F}(\underline{\mathbf{Y}}) + \int_{\mathcal{H}} \omega \langle \boldsymbol{\xi} \rangle \Delta \underline{Y}_i \langle \boldsymbol{\xi} \rangle \xi_p K_{pj}^{-1} dV_{\boldsymbol{\xi}} \\
&= \mathbf{F}(\underline{\mathbf{Y}}) + \int_{\mathcal{H}} \omega \langle \boldsymbol{\xi} \rangle \Delta \underline{Y}_k \langle \boldsymbol{\xi} \rangle \delta_{ik} \xi_p K_{pj}^{-1} dV_{\boldsymbol{\xi}} \\
&= \mathbf{F}(\underline{\mathbf{Y}}) + (\delta_{ik} \omega K_{pj}^{-1} x_p) \bullet \Delta \underline{Y}_k \quad (\text{from Equation F.3})
\end{aligned} \tag{F.18}$$

where, δ_{ik} is the Kronecker delta having the properties:

$$\delta_{ik} = \begin{cases} 1 & i = k \\ 0 & \text{otherwise} \end{cases} \tag{F.19}$$

Now using the definition of the Fréchet derivative we can, by inspection, see the following:

$$\nabla F_{ijk}(\underline{\mathbf{Y}}) = \delta_{ik} \omega K_{pj}^{-1} x_p \tag{F.20}$$

Now let us compute the incremental change in $\hat{W}$ due to an incremental change in $\underline{\mathbf{Y}}$ starting from Equation F.16 we have the following:

$$\Delta \hat{W} = \frac{\partial \Omega}{\partial F_{ij}} \Delta F_{ij} \tag{F.21}$$

If we rearrange Equation F.18 slightly we can see the following relationship:

$$\Delta F_{ij} = \mathbf{F}(\Delta \underline{\mathbf{Y}}) = (\delta_{ik} \omega K_{pj}^{-1} x_p) \bullet \Delta \underline{Y}_k \tag{F.22}$$

Substituting Equation F.20 into Equation F.22 and that result into Equation F.21 yields Equation F.23.

$$\Delta \hat{W} = \frac{\partial \Omega}{\partial F_{ij}} \nabla F_{ijk} \bullet \Delta \underline{Y}_k \tag{F.23}$$

Recall that the first Piola-Kirchhoff stress, $\boldsymbol{\sigma}$, is related to the strain energy density through the tensor gradient,

$$\sigma_{ij}(\mathbf{F}) = \frac{\partial \Omega}{\partial F_{ij}}(\mathbf{F}) \tag{F.24}$$

Substitute Equation F.24 into Equation F.23 to get the following:

$$\Delta \hat{W} = \sigma_{ij} \nabla F_{ijk} \bullet \Delta \underline{Y}_k \tag{F.25}$$

$$= (\sigma_{ij} \delta_{ik} \omega K_{pj}^{-1} x_p) \bullet \Delta \underline{Y}_k \tag{F.26}$$

$$= (\sigma_{kj} \omega K_{pj}^{-1} x_p) \bullet \Delta \underline{Y}_k \tag{F.27}$$

Finally, by comparing Equation F.27 with Equation F.7 and recalling that $\mathbf{K}$ is a symmetric tensor we can see by inspection,

$$\underline{T}_i = \sigma_{ij} \omega K_{jp}^{-1} x_p \tag{F.28}$$

or equivalently,

$$\underline{\mathbf{T}} \langle \boldsymbol{\xi} \rangle = \omega \langle \boldsymbol{\xi} \rangle \boldsymbol{\sigma} \mathbf{K}^{-1} \boldsymbol{\xi} \tag{F.29}$$

Which is the same as Equation 4.21.

G Hole in a Plate Problem

Before implementing and validating the viscoplasticity model as reported in Chapter 4 a purely elastic model was validated first. The elastic (Hooke's law) constitutive model shown in Equation G.1,

$$\tau_{ij} = 3\mathcal{K} \left(\frac{1}{3} \varepsilon_{kk} \delta_{ij} \right) + 2\mu \left(\varepsilon_{ij} - \frac{1}{3} \varepsilon_{kk} \delta_{ij} \right) \quad (\text{G.1})$$

where, $\mathcal{K}$ is the material bulk modulus, μ is the material shear modulus, τ and ε represent tensor components of stress and strain, respectively, and δ_{ij} is the Kronecker delta. This model was implemented into the peridynamic code Emu in a fashion identical to that described in Chapter 4 for the viscoplastic model (i.e., through the conversion of a stress tensor into a force-vector state description).

In order to validate our elastic constitutive model we will consider the classic problem of a small hole of radius, a , in an infinite plate, subject to a far field uniaxial tension, S illustrated in Figure G.1. This problem has an exact solution of the field equations. The

Figure G.1: Illustration of infinite plate with small hole.

components of stress in polar coordinates are shown in Equation G.2 through Equation G.4.

$$\tau_{rr}[r, \theta, S] = \frac{S}{2} \left(1 - \frac{a^2}{r^2} \right) + \frac{S}{2} \left(\frac{3a^4}{r^4} - \frac{4a^4}{r^2} + 1 \right) \cos(2\theta) \quad (\text{G.2})$$

$$\tau_{\theta\theta}[r, \theta, S] = \frac{S}{2} \left(\frac{a^2}{r^2} + 1 \right) - \frac{S}{2} \left(\frac{3a^4}{r^4} + 1 \right) \cos(2\theta) \quad (\text{G.3})$$

$$\tau_{r\theta}[r, \theta, S] = \frac{S}{2} \left(\frac{3a^4}{r^4} - \frac{2a^2}{r^2} - 1 \right) \cos(2\theta) \quad (\text{G.4})$$

Obviously, there is no way to numerically simulate an infinite plate, but we can approach the solution if we make the plate size many times the diameter of hole. In this case the plate was made to be 10 times, in length and width, the diameter of the hole. The peridynamic model does not allow use to apply a far field stress as a boundary condition; therefore, a little creativity was required in order extract the information needed to make a meaningful comparison to the exact solution. A constant velocity was applied to a volume of nodes along two edges of the plate in opposite directions. The resulting stress in the plate was then normalized by the stress recorded in those nodes that the velocity was applied to. Two interesting comparisons we can make to the exact solution are shown in Figure G.2 and Figure G.3. If we evaluate Equation G.3 at $r = a, \theta = \pi/2$ with an applied far field stress $S = 1$ we get the result shown in Equation G.5.

$$\tau_{\theta\theta}[a, \pi/2, 1] = 3 \quad (\text{G.5})$$

Comparing the result from Equation G.5 with the location of evaluation in Figure G.2 we can see very good correlation between the peridynamic simulation and the exact solution. We can also evaluate Equation G.4 at $r = a, \theta = \{0, \pi/2, \pi, 2\pi\}$ with an applied far field stress $S = 1$, the result is shown in Equation G.6:

$$\tau_{\theta\theta}[a, \{0, \pi/2, \pi, 2\pi\}, 1] = 0 \quad (\text{G.6})$$

Comparing the result from Equation G.6 to Figure G.3 at each of the evaluation locations we can see that the numerical simulation compares well with the exact solution.

One final comparison was done by looking at the $\tau_{\theta\theta}$ stress along the line $\theta = 0, r$. The Emu simulations were run at two different node densities labeled course and fine in Figure G.4. The course node density represented 20 nodes across the diameter of the hole and the fine node density corresponded to 40 nodes across the diameter of the hole. The simulations were run in order to see if the peridynamic stress measurements converged. Figure G.4 shows no difference in the values of stress between the two simulations. They both compare well with the exact solution as well. Small differences between the exact solution and the simulations are to be expected because the exact solution is for an infinite plate and the simulations are clearly done on a finite plate. Overall these simulations validated the elastic peridynamic model and gave us the confidence to proceed with the implementation of the viscoplastic model.

Figure G.2: Normalized Cauchy stress, $\tau_{\theta\theta}$.

Figure G.3: Normalized Cauchy stress, $\tau_{r\theta}$.

Figure G.4: Normalized stress as a function of distance along $\theta = 0, r$ axis.

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