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Peridynamic models for fatigue and fracture in isotropic and in polycrystalline materials

Guanfeng Zhang
gzhang@Huskers.unl.edu

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PERIDYNAMIC MODELS FOR FATIGUE AND FRACTURE IN ISOTROPIC AND IN
POLYCRYSTALLINE MATERIALS

by

Guanfeng Zhang

A DISSERTATION

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PERIDYNAMIC MODELS FOR FATIGUE AND FRACTURE IN ISOTROPIC AND IN
POLYCRYSTALLINE MATERIALS

Guanfeng Zhang, Ph.D.
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Adviser: Florin Bobaru

To improve design and reliability, extensive efforts has been devoted to understanding
damage and failure of materials and structures using numerical simulation, as a complement
of theory and experiment. In this thesis, peridynamics is adopted to study fatigue and
dynamic failure problems.

Fatigue is a major failure mode in engineering structures. Predicting fracture/failure
under cyclic loading is a challenging problem. Classical model cannot directly be applied
to problems with discontinuities. A peridynamic model is adopted in this work because of
important advantages of peridynamics in allowing autonomous crack initiation and propagation.
A recently proposed peridynamic fatigue crack model is considered and improved in terms
of computational efficiency and numerical stabilities. We validated the fatigue crack model
by comparing simulation results of a modified compact tension test with experiments. The
proposed improvements add the fatigue limits to the propagation phase. We demonstrate
that the model simulates all three phases of fatigue failure (initiation, propagation, and
final failure) with an example in which a fatigue crack sinks into a cutout and re-initiates
from a different location along the cutout, grows, and lead to final failure of the structure.
Convergence studies show that the peridynamic results are correct once the nonlocal size is
smaller compared with the size of relevant geometrical features.

In the second part of this thesis, a 3D peridynamic model for cubic crystalline elastic and
brittle materials is proposed. We use the model to simulate the Edge-on impact test of a
transparent ceramic material, AlON. Experiments show that in ALON, damage transitions from a fast failure front (faster than the shear wave in the sample) to much slower localized cracks. Using the peridynamic model we explain, for the first time, the reasons behind this transition, and why failure front moves faster than the shear wave speed in the material. We also use the polycrystalline peridynamic model to predict crack nucleation sites in a Ni-based superalloy. Peridynamic results for a synthetic polycrystalline sample under tension are compared with finite element simulations. Results show that the model introduced captures the strain distribution and all strain concentration sites predicted by the FEM model, and in addition, it allows for initiation, growth, and interactions of cracks.
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Chapter 1 Introduction

1.1 Motivation and objective

Peridynamics, a new non-local method, has been proposed to deal with dynamic fracture problems by Silling [1]. Peridynamics is a reformulation of the classical continuum mechanics equations that allows for a natural treatment of discontinuities in the solution by employing the concept of nonlocal interactions. Integration, rather than differentiation, is used to compute the total force density acting on a certain material volume, and deformation gradients are not used in the formulation [2]. A distinguishing feature of the peridynamic approach is that it allows for spontaneous formation, interaction, and growth of discontinuities in a consistent framework [3].

Finite element method (FEM) or various modified versions of the FEM are the most popular computational methods to simulate damage and failure under both static and dynamic loadings. Existing FEM models are based on the classical continuum mechanics equations, which are described by partial differential equations. In order to solve problems with discontinuities, such as cracks, special techniques need to be devised. Most of these techniques essentially treat every new configuration as a problem in a new domain, since the crack creates new surface and the boundaries of the initial domain change. This requires tracking of the crack surface in some way. Other complications relate to describing crack initiation, to determining direction of propagation, and the speed of propagation. All of these aspects require laws of propagation (or “kinetic relations”) and most of the time they are setup in an ad-hoc manner: they may work for one example, but not for another. For
example, popular criteria used in FEM and XFEM for guiding the crack growth are: the maximum circumferential stress criterion (MCSC) (see [4]), the maximum strain energy release rate criterion (MSERRC) (see [5]), the minimal strain energy density (MSEDC) (see [6]), and the material forces criterion (MFC) (see [7]). These criteria have been tested and compared in 3D simulations based on XFEM ([8]). Results show that the MSEDC and the MFC have considerable problems for torsion, and only the MSERCC is able to provide meaningful results for mixed mode I/II/III. These criteria can only used to calculate the crack growth direction, additional criteria are needed for other crack behaviors, like crack branching or coalescence.

One of the simplest methods to modeling propagating cracks is the element-deletion (also known as “element-erosion”) method. Such methods suffer from nonconvergence in the limit of the mesh size going to zero. Recent improvements of these approaches have been produced using variational formulations ([9]) or nonlocal averaging of displacement gradients schemes (see [10]) as those employed in the nonlocal models of Eringen [11]. The results in [9] match well quasi-static type of crack growth under mixed-mode conditions. While a length-scale is introduced in the element erosion model of [9] in order to regularize the problem and insure convergence in the limit of the mesh being refined, it is not yet known how this method performs in the crack branching problem.

Alternatives to element-erosion techniques are cohesive zone FEM models (see e.g. [3, 12]). Such models remove the need of pre-knowledge of the crack path. The crack path, however, is still forced to follow the particular mesh used, since cracks can only propagate along the element boundaries ([13, 12, 14]). Since the correct, actual crack path (which minimizes the strain energy) of the propagation process is not computed correctly, there are significant departures from the true energy released during the crack propagation event. In such cases, reliable prediction of strength of brittle ceramics under impact, for example, becomes difficult. The XFEM [15] allows cracks to pass through the finite elements leading to
better approximations of the crack path. Interestingly, in dynamic brittle fracture problems, one may need to drastically modify the input fracture energy in the model in order to obtain crack propagation speeds similar to those seen in experiments (see [16]). Subdivision of the cut elements for numerical integration purposes increases the complexity and the cost of the method and the method requires phenomenological damage models and branching criteria as input, and requires tracking of the crack path, for example, using level sets. A recent review of methods that use tracking of the crack path has been recently provided in [17].

Using peridynamic simulation, promising results have been obtained in, for example, dynamic brittle fracture in glass [18, 19, 20], fiber-reinforced composites [21]), functionally graded materials [22], pitting corrosion damage [23, 24], flow in porous media [25], and coupling with continuum based method [26, 27]. Most published applications of peridynamics focus on dynamic fracture simulations. Fatigue is a major failure mode in engineering structures, the application of peridynamics in this area would benefit the simulation of complex fatigue cracking problems, like fatigue crack of composites. In 2010, The first peridynamic fatigue failure model [28] was proposed, which decreases the critical stretch of peridynamic bonds as loading cycle increases. One major limitation of this model is that it can only be used to simulate the crack growth phase. In 2014, another peridynamic model for fatigue cracking was proposed by Silling and Askari [29], which enables the simulation, in a single model, of the three phases of fatigue failure: crack initiation, fatigue growth and final failure controlled by quasi-static crack growth. The first part of this dissertation validates this model by comparing with experimental and finite element results on a benchmark problem and extends this peridynamic fatigue crack model. The extended model is able to continue the simulations through full failure of the sample, and we observe the expected large rotations of the sample past final failure.

The second part of this dissertation focuses on simulating failure and damage of a polycrystalline ceramic, AlON. Combined transgranular (cracks pass through the grains) and
intergranular (cracks propagate between the grains) fracture can happen in brittle fracture of ceramics [30]. Existing models [31, 13] for simulating brittle fracture in polycrystalline ceramics that can include combined trans- and inter-granular crack propagation have severe limitations, including: the inability of modeling propagating cracks that naturally coalesce and/or branch; limitation to modeling only a single or just a couple of cracks; complicated algorithms that cannot extend to 3D, etc. Compared to existing methods, the cubic elasticity model based on peridynamics [1, 32] used here for analyzing crack initiation, propagation, and fragmentation in a rate-dependent mechanically loaded Voronoi polycrystalline ceramics has important advantages because: a) The cracks initiate and propagate when and where is it energetically favorable to do so [20]; b) Inter- and transgranular fracture are direct consequences of the computations and they do not have to be postulated via ad hoc assumptions as is the case for the classical approach [33]; c) Mode-transition and mode-mixing of crack propagation is naturally captured by the peridynamic formulation [18, 19, 21]; d) Fracture at triple-junction points is not controlled by ad-hoc assumptions but by the actual loading conditions in the region surrounding the triple-junctions [33]; e) Complex interaction between cracks does not have to be assumed, but rather it is part of the solution [21, 20]; f) The meshfree character eliminates the need for complex meshing algorithms of Voronoi polycrystals. The peridynamic model captures the the failure procedure observed in experiments: fast coherent damage front, followed by development of slower distinct “radial” trans- and intergranular cracks. Also, the peridynamic results match well the final damage pattern on the sample surface, and propagation speeds of both the damage front, and of the subsequent radial cracks. The damage mechanism of the Edge-on impact is proposed based on simulation results.

At last the peridynamic cubic elasticity model is used to predict crack nucleation sites in a superalloy, René 88DT. Understanding of the crack nucleation stage and incorporating microstructure in design are still in elementary stage [34]. Experimental work [35] shows that
most crack nucleated near the Σ3 twin boundaries in surface grains with size three times larger than average grain size because larger grains allow more slip transmission. Crystal plasticity is capable of capturing the heterogeneous plastic deformation, texture evolution, and dislocation of metallic material under large deformation. Coupling crystal plasticity with finite element method is the most popular approach for understanding microscopic plastic deformation and crack nucleation. The challenge of using

1.2 Thesis outline

The outline of this thesis is as follows:

- chapter 2 reviews basic formulations for bond-based peridynamics, including equations of motion, equations for calibrating micromodulus by matching elastic constants in a classical continuum, and the equation for calibrating critical bond stretch.

- chapter 3 reviews the peridynamic fatigue crack model and provides details of numerical implementation: obtaining the static solution in peridynamics by energy minimization, the peridynamic J-integral. A set of critical damage factors is proposed to maintain the computational stability and improve efficiency. A GPU-based acceleration method is provided, and promising speed up is obtained. We validated the fatigue crack model against experiments, predicted fatigue crack paths and fatigue lives match with experiments very well. An extension is proposed because the original fatigue crack model ignored the Paris’ law is not valid when the stress intensity range is smaller than its threshold. The issues are explained by simulating a modified compact tension test. In addition, three phases of fatigue failure are shown using the extended model. Results demonstrated the effectiveness of the proposed extension. This chapter has been published [36, 37].
• chapter 4 proposes a peridynamic cubic elastic model. We provide numerical implementation detail, perform numerical studies, and use this model to simulate an Edge-on impact test of AlON. Simulation captures the failure mode observed in experiments, transitions from perfusive damage and transgranular fracture. We conclude that elastic anisotropy, material microstructure, and brittle failure are the main ingredients that determine the evolution of damage in polycrystalline AlON.

• chapter 5 uses the cubic elastic model to predict the crack nucleation sites in a Ni-based superalloy. We perform three verification case studies, effective modulus variation in single grain with different orientations, strain variation across a grain boundary, and strain concentration sites in a complex polycrystalline model. Results show that this model can predict the crack nucleation sites under fatigue loading.

• chapter 6 concludes the dissertation and discusses future work. For each topic, detailed backgrounds are provided at the beginning of each chapter.
Chapter 2 Peridynamic theory

Peridynamics is a reformulation of the classical continuum mechanics equations that allows for a natural treatment of discontinuities in the solution by employing the concept of nonlocal interactions [1]. Integration, rather than differentiation, is used to compute the total force density acting on a certain material volume, and deformation gradients are not used in the formulation. Peridynamics differs from other nonlocal methods such as those described by Eringen [11], Kunin [38], and Rogula [39], or those reviewed by Bažant and Jirásek in [40], for at least two fundamental reasons:

1. The deformation gradient and strains (spatial derivatives of displacements) are not used in peridynamics. Other nonlocal methods average strains over the nonlocal region. Spatial derivatives of the displacement field become undefined when discontinuities, like cracks, emerge and this requires special treatment and algorithms in models that employ such derivatives in their formulation.

2. Damage is introduced in the peridynamic method at the microlevel in the constitutive model for the peridynamic bonds between material points. When the relative elongation of the bond reaches a failure criterion related to the material’s fracture energy, the bond breaks. Fracture surfaces result autonomously as a consequence of this definition and dealing with multiple interacting cracks of arbitrary shapes in complex geometries becomes as easy as dealing with a single straight crack. In this way, peridynamics integrates damage and fracture under a single model for material failure.
2.1 Peridynamic formulation

The peridynamic equations of motion at a point \( x \) and time \( t \) are ([1]):

\[
\rho(x)\ddot{u}(x, t) = \int_{H_x} f(u(\hat{x}, t) - u(x, t), \hat{x} - x) \, dV_{\hat{x}} + b(x, t) \quad \text{for} \quad x \in \Omega \quad \text{and} \quad t \in [t_0, \infty) \tag{2.1}
\]

where \( \Omega \) is the domain occupied by the body, \( t_0 \) is some initial time, \( u \) is the displacement vector field, \( b \) is the body force intensity, and \( f \) is the pairwise force function in the peridynamic bond that connects material points \( \hat{x} \) and \( x \). The integral is defined over a local region \( H_x \) called the horizon region, or simply the horizon. It is natural to consider the horizon as a small sphere (disk in 2D, interval in 1D) centered at the current point. We will call the radius of the sphere \( \delta \) and refer to it also as the horizon. From the context it will always be clear whether we refer to the region or its radius when we mention the word “horizon”. A discussion on the meaning, selection, and use of the peridynamic horizon and its relation to crack branching in brittle materials has appeared in Ref. [41].

For a microelastic material [1], a pairwise potential exists such that

\[
f(\xi, \eta) = \frac{\partial \omega(\xi, \eta)}{\partial \eta}, \tag{2.2}
\]

where \( \xi = \hat{x} - x \) is the relative position and \( \eta = u(\hat{x}, t) - u(x, t) \) is the relative displacement between points \( \hat{x} \) and \( x \). A linear microelastic material is defined by a micropotential \( \omega \) as:

\[
\partial \omega(\eta, \xi) = \frac{c(\xi)s^2\|\xi\|}{2}, \tag{2.3}
\]
where the \( c(\xi) \) is the micromodulus function and

\[
s = \frac{\| \eta + \xi \| - \| \xi \|}{\| \xi \|}
\]

is the relative elongation of the bond connecting \( \hat{x} \) and \( x \). For a horizon region with spherical symmetry, the corresponding pairwise force becomes:

\[
f(\xi, \eta) = \begin{cases} 
\frac{\eta + \xi}{\| \eta + \xi \|} c(\xi) s, & \| \xi \| \leq \delta \\
0, & \| \xi \| > \delta
\end{cases}
\]

(2.5)

Assuming a specific form of the isotropic micromodulus function \( c(\xi) = c(\| \xi \|) \), for example constant over the horizon region or varying linearly with \( \| \xi \| \) (see Fig. 2.1), one can find the parameters in these representations by calibrating the strain energy density computed with peridynamics to the classical strain energy density for a homogeneous deformation like equal bi-axial strain. The calibration is made for a point in the bulk, at least a distance \( \delta \) away from the boundaries so that the node has a complete horizon region. Materials points close or on the boundaries of domain \( \Omega \) have horizon regions that are partial disks. If one performs the calibration for these points, the resulting micromodulus value for the bonds connected to such points will be higher than that obtained for the points in the bulk. When the special calibration for the points within a distance \( \delta \) from a boundary is not employed, and the bond stiffness for points near the boundary is assigned to be the same as that for nodes in the bulk, the effective material behavior near the boundaries is slightly softer than in the bulk. As the horizon \( \delta \) decrease to zero, the thickness of this softer zone decreases and becomes negligible. More on this “skin effect” is discussed in [19]. To reduce, or in some cases eliminate, the surface effect, for any horizon size, at least two options have been proposed in the literature:
• introduce ghost nodes ([42]) (also called fictitious nodes, see [43]) outside of the domain. This approach may become cumbersome for bodies with complex geometries.

• compute an approximate correction of the micromoduli for nodes on or near the surface (see, for example, section 4.2 in [44]). This approach is exact only for regular boundaries and some simple homogeneous deformations.

In anisotropic materials the micromodulus function \( c(\xi) \) is defined by at least two parameters, and various ways to calibrate the models have been proposed (see [3, 45, 21, 46, 47, 48]).

For examples of micromodulus functions in 3D see [49], in 2D see [18], and in 1D see [50]. Because of its faster convergence properties to the classical elasticity solutions (as the horizon goes to zero), for the 2D conical micromodulus (see Fig. 2.1) with the plane stress assumptions:

\[
c(\xi) = C_1 \left(1 - \frac{\|\xi\|}{\delta}\right) = \frac{24E}{\pi \delta^3 (1 - \nu)} \left(1 - \frac{\|\xi\|}{\delta}\right)
\]  

where \( E \) is Young’s modulus and \( \nu \) is the Poisson ratio (fixed to 1/3 in this 2D case).

![Figure 2.1: The conical micromodulus function](image)

For 3D case, the conical micromodulus function is:

\[
c(\xi) = \frac{30E}{\pi \delta^4 (1 - 2\nu)} \left(1 - \frac{\|\xi\|}{\delta}\right)
\]  

(2.7)
To introduce damage, a law for bond failure has to be established. In peridynamics, bonds can break irreversibly ([51]), or reversibly (see [52]) when they are meant to represent Van der Waals-like interactions, for example. Here we assume irreversibility of bond breaking, thus:

\[
f(\xi, \eta, x, t) = \begin{cases} 
  f(\xi, \eta, x) & \text{if } s(\xi, x, \tilde{t}) < s_0, \text{ for all } 0 \leq \tilde{t} \leq t, \\
  0 & \text{otherwise}
\end{cases}
\]  

(2.8)

where \(s_0\) is the critical value of bond relative elongation for breakage. When a bond reaches this critical value, the break is irreversible and the bond no longer sustains a force. This critical value, which could be made to depend on the bond length \(\xi = \|\xi\|\) or on the state of local damage, for example, is defined by matching the fracture energy \(G_0\) of the material to the energy required by the peridynamic model at a point in the bulk to completely separate a body in two at that point with a fracture surface. This separation requires breaking all bonds that initially connected points on opposite sides of the fracture surface.

![Figure 2.2: Evaluation of fracture energy \(G_0\) (except from [49])](image)

In 3D, the connection between the critical relative elongation and the material fracture
energy is given by [49]

\[ G_0 = 2 \int_0^\delta \int_0^{2\pi} \int_0^{\cos^{-1}(z/\xi)} \left[ \frac{c_s^2}{2} \right] \xi \xi^2 \sin(\phi) \ d\phi \ d\theta \ d\xi \ dz \]  

(2.9)

The integration is illustrated by Fig. 2.2, which is the integral using a spherical coordinate system centered at A. The critical bond stretch is

\[ s_0 = \sqrt{\frac{5G_0}{3k\delta}}, \]  

(2.10)

where \( k \) is the bulk modulus. For the conical micromodulus functions, the critical relative elongation is obtained as:

\[ s_0 = \sqrt{\frac{2\pi G_0}{9k\delta}}. \]  

(2.11)

In 2D, the integration of fracture energy in peridynamic given by (see, e.g. [18]):

\[ G_0 = 2 \int_0^\delta \int_0^\delta \int_0^{\cos^{-1}(z/\xi)} \left[ \frac{c_s^2}{2} \right] \xi \xi^2 \sin(\phi) \ d\phi \ d\theta \ d\xi \ dz \]  

(2.12)

Using the conical micromodulus functions, the critical relative elongation is obtained as:

\[ s_0 = \sqrt{\frac{5\pi G_0}{9E\delta}}. \]  

(2.13)

Similar to “skin effect” discussed above for the computation of the micromodulus function, the critical relative elongation \( s_0 \) value is affected near the boundary of the domain, or in a region where damage is already present. This happens because the above calculation is based on points in the bulk. For points on or near the boundary, the domain of integration is smaller, and when matched to the same \( G_0 \) value, the resulting critical relative elongation would be higher than in bulk. Therefore, when a constant \( s_0 \) computed for a point in the bulk is used in computations, the peridynamic material model will effectively have slightly weaker
bonds for points near the surface than for those in bulk. The same happens in regions where damage is present, such as on the surface of a propagating crack. As the horizon goes to zero, the weaker “skin” region goes to zero, and the effect is minimized. Some attempts to correct this for regions where damage is present have been implemented in the code EMU ([53]) and showed better results in fragmentation problems. The correction, also discussed and used in [19], consists in increasing, in an approximate way, the value of the $s_0$ for points with a certain amount of damage, proportional to the damage amount. This model is referred to as the “damage-dependent peridynamic model”.
Chapter 3  Modeling the evolution of fatigue failure with peridynamics

A peridynamic model for fatigue cracking is proposed by Silling and Askari [29], which enables the simulation, in a single model, of the three phases of fatigue failure: crack initiation, fatigue growth and final failure controlled by quasi-static crack growth. In [29], dynamic relaxation method is used to obtain the static solution, and fatigue crack growth is demonstrated by using a standard compact tension test and torsional load on a rod. In the present work, the static solution is obtained by using the conjugate gradient energy minimization method, which is matrix-free and hundreds times faster than dynamic relaxation method (see [54]). We also introduce a set of two critical damage parameters that improve computational efficiency and maintain stability in the numerical solution process. The range for these parameters is determined via convergence studies of fatigue crack growth for a standard compact tension (CT) test. We then test the peridynamic fatigue crack model for curved fatigue crack growth by using modified CT tests, in which the location of a hole determines whether the crack sinks into it or by-passes it. The peridynamic simulation results demonstrate that accurate path prediction and life prediction in arbitrary 2D geometries can be obtained.

The advantage of the peridynamic fatigue crack model compared to those based on classical continuum mechanics is also evidenced by another example of fatigue crack growth in a composite material. The peridynamic fatigue crack model does not require additional criteria to guide crack growth. We use the peridynamic fatigue crack model, without any modifications, to simulate fatigue crack growth in a two-phase composite in which several crack initiation points exist and where fatigue crack paths interact in complex ways.
Holes and round notches are locations where fatigue cracks may arrest. Investigating the evolution of fatigue cracks after sinking into such a hole is important. Here we extend the crack peridynamic model to treat such cases. The proposed improvements add the fatigue limit to the propagation phase. We demonstrate that the model simulates the three phases of fatigue failure (initiation, propagation, and final failure) with an example in which a fatigue crack sinks into a cutout and re-initiates from a different location along the cutout, grows, and lead to final failure of the structure.

3.1 Peridynamic model for fatigue cracking

Recently, a peridynamic model for fatigue cracking was introduced in [29] for linear isotropic materials. This was the first time that a single model can simulate three phases in fatigue failure: crack initiation, crack propagation, and final failure controlled by quasi-static crack growth. In this section we briefly review the main components of this model, with slight differences in the notations used.

The main difference between the peridynamic elastic-brittle model shown in the previous section and the peridynamic model for fatigue cracking is in the damage model. The Eq. (2.8) is replaced by:

\[
f(\xi, \eta, x, \lambda, t) = \begin{cases} 
  f(\xi, \eta, x, \lambda) & \text{if } s(\xi, x, \tilde{t}) < s_0 \text{ and } \lambda < 0 \text{ for all } 0 \leq \tilde{t} \leq t, \\
  0 & \text{otherwise}
\end{cases}
\]  

in which \( \lambda \) is a damage variable called the bond “remaining life”, that evolves over time with the number of fatigue cycles. The remaining life is unity for intact bonds, and it is monotonically decreasing over the number of cycles. A bond fails at the first cycle \( N \) when \( \lambda(N) \leq 0 \).

In [29], Silling and Askari introduce the evolution law for the remaining life and calibrate
it with S-N curve data for the fatigue crack initiation phase, and with Paris’ law data for modeling of the fatigue crack propagation phase. The final failure phase is accounted for by the critical bond strain $s_0$ (see Eqs. (2.10, 2.13)) discussed in the previous section.

The starting point of the model is the following evolution law for the remaining life of a bond:

$$\frac{d\lambda}{dN}(N) = -A\varepsilon^p. \tag{3.2}$$

where $\varepsilon = |s_{\text{max}} - s_{\text{min}}|$ is the current cyclic strain range in the bond, $s_{\text{max}}$ and $s_{\text{min}}$ are the maximum and minimum bond strains in this cycle, and $A$ and $p$ are positive constants to be determined by calibration to experimental results, separately: $A_1, p_1$ from first phase of fatigue cracking, and $A_2, p_2$ from the second phase of fatigue cracking.

Because the material behavior is assumed to be linear, the cyclic bond strain range can be expressed by $s_{\text{max}}$ and load ratio $R = s_{\text{min}}/s_{\text{max}}$:

$$\varepsilon = |s_{\text{max}} - s_{\text{min}}| = |(1 - R)s_{\text{max}}| \tag{3.3}$$

In this way, only the maximal loading case is needed in simulations.

For the fatigue crack nucleation phase (phase I), calibration is performed by integrating the evolution law in Eq. (3.21) from the zero-th cycle to the cycle at which the first bond breaks, and enforcing a match between the equation of the straight line obtained in the log-log plot from the integration procedure and a corresponding straight line obtained, by some linear fit, from an S-N curve in strains (see Fig. 3.1).

Considering the first bond in the entire domain $\Omega$ that breaks from fatigue loading, and denoting by $\varepsilon_1$ its cyclic strain range, we integrate Eq. (3.21) as mentioned above to obtain:

$$A_1\varepsilon_1^{p_1}N_1 = 1 \tag{3.4}$$
where \( N_1 \) is the smallest cycle at which this bond breaks, meaning \( \lambda(N_1) = 0 \) for this bond.

In log-log, this represents the equation of a straight line, and the two parameters \( A_1 \) and \( p_1 \) are found by enforcing the match between this straight line and a similar straight line coming from an S-N curve in terms of strains (see Fig. 3.1). Once \( A_1 \) and \( p_1 \) are found, we can compute \( N_1 \) needed for first nucleation. Notice that here we assume that the cyclic strain range is independent of the cycle number \( N \). Therefore, the first bond breaks in phase I when its fatigue cycle number \( N \) becomes larger than \( N_1 \):

\[
N \geq \frac{1}{A_1 \varepsilon_1^{p_1}}. \tag{3.5}
\]

When at least one bond with cyclic bond strain range \( \varepsilon_1 \) breaks in phase I, a new static solution is calculated at the same cycle; strains are going to increase in nearby bonds. If these bond strain ranges are larger than \( \varepsilon_1 \), the bonds are broken and iterations of the static solution continue at the same cycle until no more bonds break. The computations continue with the next fatigue cycle number. The new fatigue cycle number is larger than \( N_1 \), and so bonds with \( \varepsilon > \varepsilon_1 \) will break. At this fatigue cycle, the static solutions iterations are used.
as above.

Phase I fatigue damage switches to phase II (fatigue crack growth) at a certain node if the node has, within its horizon (including itself), a node with damage \( d \geq 0.5 \). At this stage, one or more initiated fatigue cracks exist in the sample. Notice that if a pre-crack is present in the sample, there already are nodes with this damage property \( (d \geq 0.5) \) and they would directly switch to phase II. Note also that the reset, indicated in [29], of the remaining life for bonds connected to the nodes that switch to phase II is not necessary because the fatigue life of such intact bonds is still equal to one at the end of phase I.

In the fatigue crack growth phase (phase II), the value of remaining life \( \lambda_{i,j}^n \) of a bond, which connects nodes \( x_i \) and \( x_j \), evolves according to the Eq. (3.21). With a discretization of the range of cycle numbers, \( N(0), N(1), \ldots, N(n), \ldots \), and using backward finite differences to discretize the bond remaining life equation we get:

\[
\lambda_{i,j}^0 = 1, \quad \frac{\lambda_{i,j}^n - \lambda_{i,j}^{n-1}}{N(n) - N(n-1)} = -A_2(\varepsilon_{i,j}^n)^{p_2}
\]

(3.6)

where \( \varepsilon_{i,j}^n \) is the cyclic bond strain at step \( n \). If we knew \( A_2 \) and \( p_2 \), Eq. (3.6) would allow us to compute the remaining life at the current step, \( n \). This will then lead to a particular crack growth rate.

To determine the two parameters \( A_2 \) and \( p_2 \), we perform calibration by enforcing a match between the peridynamic crack growth rate with that from Paris’ law, which is experimentally obtained. Along with [29], we assume constant crack growth rate in each loading cycle. The evolution law for the remaining life of a bond only works for bonds within the horizon of a node that is in phase II fatigue cracking, near a phase I-initiated crack tip or a pre-crack tip. The peridynamic crack growth rate derived in [29] is:

\[
\frac{da}{dN}(N) = \beta A_2 \varepsilon_{core}^{p_2}
\]

(3.7)
where $\varepsilon_{\text{core}}$ is the cyclic bond strain range of the core bond (see Fig. 3.2). The core bond is the bond with the largest maximum strain in front of the crack tip. The parameter $\beta$ represents the geometry influence on the strain distribution. For the detailed derivation of this formula please see [29].

On the other hand, Paris’ law [55] is:

$$\frac{da}{dN}(N) = c\Delta K^M, \quad (3.8)$$

where $c$ and $M$ are constants determined from experiments, and $\Delta K$ is the stress intensity range. By enforcing the match between Eqs. (3.7) and (3.8), we can set $p_2 = M$, because the stress intensify factor is proportional to strain.

To determine $A_2$, since $\beta$ is not known in closed form, we need to find an alternative route. We can perform a single peridynamic simulation of fatigue crack growth with an arbitrary value of $\hat{A}$ and the already calibrated $p_2$ value. Eq. (3.6) allows us to compute the current remaining life, and therefore, these calculations produce a certain crack growth rate, call it $(da/dN)$. Because the crack growth rate $da/dN$ depends linearly on $A_2$, we can then compute the Paris law-calibrated value for $A_2$ as follows:

$$A_2 = \hat{A} \frac{da/dN}{(da/dN)} = \hat{A} \frac{c\Delta K^M}{(da/dN)}. \quad (3.9)$$

Another available fatigue failure model is provided in [28], in which the critical stretch of peridynamic bonds decreases as loading cycle increases. One major limitation of this model is that it can only be used to simulate the crack growth phase. As discussed before, a model that can simulate crack initiation, growth and final failure is critical for fatigue crack modeling because of the complexities and changes in stress distribution in the evolution of material damage due to fatigue loading. That is why the fatigue cracking model in [29] is
3.2 Numerical implementation

In this section we describe the numerical implementation details related to the peridynamic fatigue cracking model. As shown in a flowchart in Fig. 3.3, peridynamic simulation of fatigue cracking starts from initialization (mesh generation, family search, and boundary conditions application), solving static problems, followed by fatigue crack (includes crack nucleation phase and crack growth phase) and/or static crack growth simulation. Because previous section discussed the bond damage in three phases, this section focuses on the numerical implementation for solving peridynamic static problems, calculating the peridynamic J-integral and stress intensity factor K. More importantly, we introduce a new set of critical damage factors to improve the numerical stability and efficiency of the peridynamic fatigue crack model.
3.2.1 Static solution in peridynamics

Static analysis is the basis of peridynamic fatigue simulation. Most published applications of peridynamics focus on dynamic fracture simulations. These simulations usually use explicit time integration which require a conservative time step to maintain numerical stability. A stable time step can be in the range of microseconds or smaller, depending on the longitudinal wave speed in the sample undergoing dynamic brittle fracture. Such calculations are prohibitively costly for fatigue processes that can last hours, days, or more. Therefore, an implicit solver is needed for fatigue simulations. There are three options to get implicit solutions for quasi-static elasticity and crack-growth based on peridynamics:

- In [56], Macek and Silling proposed a method to couple peridynamics with FEM, thus
nodal displacement can be solved similar to FE technique by assembling the stiffness and mass matrices and solve the resulting systems of equations;

- Kilic and Madenci [57] used the adaptive dynamic relaxation method, by applying a viscous force to dissipate the kinetic energy of the system. A static state can be achieved after a sufficiently long time;

- In [54, 58], the energy minimization method was used (conjugate gradient solver) to find the equilibrium state, when the total potential energy of the system is minimized.

The peridynamic static equation is obtained by setting the acceleration term to zero in Eq (2.1)

$$\int_{H_\mathbf{x}} \mathbf{f}(\mathbf{u}(\mathbf{x}, t) - \mathbf{u}(\mathbf{x}, t), \dot{\mathbf{x}} - \mathbf{x}) dV_\mathbf{x} = 0 \quad \text{for } \mathbf{x} \in \Omega \quad (3.10)$$

Because the peridynamic bond force, see Eq (3.1), is nonlinear with respect to displacement $\mathbf{u}$, we cannot obtain displacement results by solving a linear algebraic equation. Considering that we can achieve the equilibrium equation using the *Euler-Lagrange Equations*, which is the derivative of strain energy to the displacement, here we use a energy minimization method [54] to solve the peridynamic static equation, the conjugate gradient (CG) method with secant line search is adopted to minimize the strain energy of the system. This method is chosen because of its advantages versus the adaptive dynamic relaxation method, which may need hundreds of times more iterations than the CG solver (see [54]). In addition, low memory requirements is an important benefit of CG in simulation of 3D fatigue cracking because it is a matrix-free solver. For all simulations in this chapter, the CG method is used with a convergence tolerance defined by: $|W_i - W_{i-1}|/W_{i-1} < 10^{-6}$, in which $W_i$, and $W_{i-1}$ are the total strain energy at current ($i$) and previous ($i - 1$) CG iterations.
Numerical simulations are performed using the discretized equation of motion:

\[
\rho_i \frac{y_i^{k+1} - 2y_i^k + y_i^{k-1}}{\Delta t^2} = \sum_{j \in H_i} f(x_j, x_i, t^k) \Delta V_j + b_i^k \quad \forall x_i \in B
\]

(3.11)

where \(i\) and \(j\) are node numbers, \(\Delta V_j\) is the reference volume of node \(j\), \(k\) is the time step, and \(\Delta t\) is the time step size. For static problems, this equation reduces to

\[
\sum_{j \in H_i} f(x_j, x_i) \Delta V_j + b_i = 0 \quad \forall x_i \in B
\]

(3.12)

Notice that node \(j\) may not be fully contained within the horizon of node \(i\), so partial volume integration is used here to improve the accuracy of mid-point quadrature scheme. The partial volume algorithm is first proposed by [59] and discussed in [60, 61]. The accuracy of this algorithm is discussed in [61].

### 3.2.2 The J-integral and the stress intensity factor

The J-integral introduced by Rice [62], as a general version of the energy release rate, provides a consistent way to characterize fracture of linear and nonlinear elastic materials. The J-integral in peridynamics is proposed by Silling [32] for 3D state-based peridynamics, and its implementation and convergence properties for 2D bond-based peridynamic model are shown in [63]. The J-integral formulation provided by [63] is used here to compute an effective stress intensity factor range which controls the fatigue crack propagation phase. Since the experimental fatigue crack growth procedure in [64] uses a constant stress intensity factor range, we use the same procedure in our peridynamic simulations, for proper validation of the fatigue model.
Figure 3.4: Integration domains for the peridynamic J-integral. The red curve is the contour of integration (from [63]).

The peridynamic J-integral formula in 2D is:

$$J_{\text{peri}} = \oint_{\partial R} W(x, a) n_1 dB - \frac{1}{2} \iint_{R_2 \cup R_3} f(\eta, \xi) \cdot \left( \frac{\partial \hat{u}}{\partial x_1} + \frac{\partial u}{\partial x_1} \right) dA_\xi dA_x$$ \hspace{1cm} (3.13)

As illustrated in Fig. 3.4, the first term in the J-integral formula is a contour integral along \( \partial R \), where \( R = R_1 \cup R_2 \). The set \( R_2 \) is a “band” of thickness \( \delta \) inside of the contour \( \partial R \), and \( R_3 \) is a band of thickness \( \delta \) outside of the contour \( \partial R \). The second term of the peridynamic J-integral is a double domain integral. When the horizon \( \delta \) goes to zero, the formulation of peridynamic J-integral coincides with the classical J-integral formula (see [63]).

With the one-point Gaussian quadrature, the above equation becomes:

$$J_{\text{peri}} \approx \sum_{n=1}^{n_{\text{contour}}} W n_1 A x - \frac{1}{2} \sum_{i=1}^{n_{\text{inner}}} \sum_{j=1}^{n_{\text{outer}}} \left[ f(u_i^1 - u_i^2, x_i^1 - x_i^2) \left( \frac{\partial u_i^1}{\partial x_1} + \frac{\partial \hat{u}_i^1}{\partial \hat{x}_1} \right) + f(u_j^3 - u_i^2, x_j^3 - x_i^2) \left( \frac{\partial u_j^3}{\partial x_1} + \frac{\partial \hat{u}_j^3}{\partial \hat{x}_1} \right) \right] A_j A_i$$ \hspace{1cm} (3.14)

where \( n_{\text{contour}} \) is the number of nodes along the integral contour \( \partial R \), \( n_{\text{inner}} \) and \( n_{\text{outer}} \) are the number of nodes in the inner region \( R_2 \) and outer region \( R_3 \) respectively (see \( R_2 \) and \( R_3 \) in...
Fig. 3.4). Note that $x$ lives in $R_2$, and $\hat{x}$ is in the family of $x$ that lives in $R_3$. The central difference scheme is used for $\partial u/\partial x_1$ and $\partial \hat{u}/\partial x_1$, for example

$$\frac{\partial u_1}{\partial x_1} \approx \frac{u_1(x_1^i + \Delta x, x_2^i) - u_1(x_1^i - \Delta x, x_2^i)}{2\Delta x}$$ (3.15)

For general loading in plane strain conditions, the relationship between the classical J-integral and the SIF is (see e.g. [65]):

$$J = K_I^2 \left(\frac{1-v^2}{E}\right) + K_{II}^2 \left(\frac{1-v^2}{E}\right) + K_{III}^2 \left(\frac{1}{2\mu}\right)$$ (3.16)

The contribution of $K_{III}$ is zero for in-plane loading cases. The combined SIF for mode I and mode II can be calculated using the J-integral as follows (see e.g. [65]):

$$K = \sqrt{\frac{JE}{(1-v^2)}}$$ (3.17)

The combined SIF is used to calculate the stress intensity range $\Delta K$ for compact tension tests in section 3.3.1, which is $K_I$ dominated.

$$\Delta K = K_{\text{max}} - K_{\text{min}}$$

$$= (1-R)K_{\text{max}}$$

$$= (1-R)\sqrt{\frac{J_{\text{max}}E}{(1-v^2)}}$$ (3.18)

in which $K_{\text{max}}$ and $K_{\text{min}}$ are maximum and minimum SIF over one cycle, and $J_{\text{max}}$ is the maximum value of the J-integral over one loading cycle (obtained when the maximum loading is applied).
### 3.2.3 Critical damage factors

In FEM fatigue crack simulations, a crack grows by a certain amount after the growth direction is determined. The crack advancement is determined by assessing the trade-off between computation time and results accuracy. Similarly, two parameters $D_{\text{min}}$ and $D_{\text{max}}$, are introduced here to improve computational efficiency and maintain numerical stability in the peridynamic fatigue crack model.

In peridynamic simulations, damage index $d_i$ is the ratio of broken bonds by total number of bonds of a node $i$. The flowchart in Fig. 3.5 shows the use of two parameters $D_{\text{min}}$ and $D_{\text{max}}$ in fatigue cracking simulations. The maximum, over the domain, damage difference at a node between the current static solution and the previous one, $\max_{x_i \in \Omega} (d_{i}^{\text{cur}} - d_{i}^{\text{pre}})$, is compared with the values of $D_{\text{min}}$ and $D_{\text{max}}$ in order to determine the action to be taken next. The purposes of introducing $D_{\text{min}}$ and $D_{\text{max}}$ are:

1. Getting correct crack paths with minimal number of static solutions to increase computational efficiency (static solution is the most time-consuming part in fatigue simulation). This is done by comparing $D_{\text{min}}$ with $\max_{x_i \in \Omega} (d_{i}^{\text{cur}} - d_{i}^{\text{pre}})$. Another static solution is not needed if $\max_{x_i \in \Omega} (d_{i}^{\text{cur}} - d_{i}^{\text{pre}}) < D_{\text{min}}$;

2. Preventing breaking of too many bonds in one iteration which can lead to numerical instabilities and/or un-physical solutions because non-equilibrated configurations get involved. If $\max_{x_i \in \Omega} (d_{i}^{\text{cur}} - d_{i}^{\text{pre}})$ is larger than $D_{\text{max}}$, we will have bond breaks for a configuration far from equilibrium. To avoid this, calculations will go back half a step (in cycle numbers) and repeat the static solution.

Parametric studies are performed to determine values of $D_{\text{min}}$ and $D_{\text{max}}$. For this purpose, a 2D sample with with a pre-crack (see [29]) is used, see Fig. 3.6. Distributed force densities are applied on nodes on top and bottom boundaries, which result in a total force $P = 1620N$ (see
Figure 3.5: Flowchart for the use of the two critical damage factors, $D_{\text{min}}$ and $D_{\text{max}}$. 

Initialization

If $N < N_{\text{max}}$ then

- Time mapping, $N = f(t)$

- If $\text{skip}_{\text{static}} = 1$ then
  - Go to last static solution
  - Update $\lambda$

- If $\max_{x \in \Omega} (d_{i}^{\text{cur}} - d_{i}^{\text{pre}}) > D_{\text{min}}$ then
  - $\text{skip}_{\text{static}} = 0$

- If $\max_{x \in \Omega} (d_{i}^{\text{cur}} - d_{i}^{\text{pre}}) < D_{\text{max}}$ then
  - $t = t + \Delta t$

Otherwise

- $\text{skip}_{\text{static}} = 1$

- Back to last static solution, and $\Delta t = \Delta t \times 0.5$

Finish
Fig. 3.6). In peridynamic simulations, $m$-convergence and $\delta$-convergence can be performed [50]. For all simulations in this chapter, the horizon factor $m = \delta / \Delta x$ is 4 and in this section $\delta = 3.2$ mm. Notice that $D_{\text{min}}$ and $D_{\text{max}}$ are only related to $m$, so parameters $D_{\text{min}}$ and $D_{\text{max}}$ determined by this parametric studies can be used in other simulations. Simulations start with a 8.5 mm pre-crack and stop after the crack tips arrive at some $3\delta$ distance from the right boundary of the sample. For different input values of $D_{\text{min}}$ and $D_{\text{max}}$, we compare crack patterns and iterations needed, to show the influence of these two parameters on results and efficiency. Results are shown in Figs. 3.7 and 3.8.

To determine the value for $D_{\text{min}}$, we set $D_{\text{max}}$ at 0.1 and use a small “time” step ($\Delta t = 1$). We implement a linear mapping between the cycle number $N$ and the “time” $t$, as follows: $N = 10 \times t$. Results with four different $D_{\text{min}}$ values are shown in Fig. 3.7. A value $D_{\text{min}} = 0.01$, means that static analysis is performed after every single bond break, since in this 2D test, under the partial-volume type quadrature mentioned in section 3.2.1, and with $\delta / \Delta x = 4$, the maximum number of nodes in the family of a given node is 68. After 1138 iterations, with $D_{\text{min}} = 0.01$, we obtain a smooth crack path. As $D_{\text{min}}$ increases, fewer static analyses are needed (250, 198, 161 iterations for $D_{\text{min}} = 0.03, 0.05, 0.07$, respectively), however, some attempts of crack “thickening” are now noticed (Fig. 3.7). This type of fatigue damage is non-physical for the material investigated here, where a flat fatigue crack surface, relative
to the sample dimensions, is expected. Based on these results, for the computational results in Section 3.3, we select $D_{\text{min}} = 0.03$, because it balances the need of accuracy with that of computational efficiency.

To determine the value of $D_{\text{max}}$, we set $D_{\text{min}}$ to 0.01 and use the same time step as above and perform several simulations with different $D_{\text{max}}$ values. We find significant difference (see Fig. 3.8) in the fatigue damage produced by various $D_{\text{max}}$ parameters. As $D_{\text{max}}$ increases from 0.1 to 0.4, the thickness of the damage region developing from the pre-crack increases dramatically. This thickening of damage happens because the time step is too large and it leads to sudden reduction of remaining life for many bonds around the crack tip. These bonds then break, but are likely to result in an un-equilibrated configuration. This is why we have to go back (using a bisection-type scheme), as many needed, to reduce the time step until this nonphysical behavior of the fatigue damage is eliminated. For the rest of the computations in this chapter we use $D_{\text{max}} = 0.1$. 

Figure 3.7: Parametric study to determine the value for $D_{\text{min}}$. Here $D_{\text{max}}$ is set to 0.1 and $m = 4$.

Figure 3.8: Parametric study to determine the value for $D_{\text{max}}$. Here $D_{\text{min}}$ is set to 0.01 and $m = 4$. 

$D_{\text{min}} = 0.01, 0.03, 0.05, 0.07$
3.2.4 GPU based acceleration

A peridynamic fatigue simulation uses repeated calls to a peridynamic quasi-static solver. The quasi-static solution, at every fictitious fatigue time step, updates the remaining life of bonds in phase I and phase II until a bond breaks because its remaining life reaches zero. A bond can also break, in phase III, if it reaches the critical bond strain criterion [49].

Given the computational cost of repeatedly solving nonlinear algebraic systems in a peridynamic simulation of fatigue crack growth, the need for parallel implementations is obvious. Options that require small changes to a serial code for this purpose are: OpenMP and OpenACC. Here we use OpenACC, a directives-based parallel programming model designed for programming massively parallel processors, to accelerate peridynamic simulations.

Similar to OpenMP, the acceleration is obtained by adding a series of derivatives. OpenACC compilers automatically map compute-intensive loops to parallel or vector execution units. An advantage of OpenACC is that it support various accelerator, like NVIDIA GPUs, AMD GPUs, and Intel MICs. Also, using PGI Accelerator, we can run Fortran code with OpenACC directives on multicore CPUs. The multicore capability breaks one limitation of GPU devices that they have much smaller memory size compared with the motherboard memory.

The pseudo code in Algorithm 1 shows the details of calculating internal forces in a peridynamic simulation. For simplicity of exposition, this sample pseudo code shows the simplest internal force calculation, that does not include the partial volume integration scheme [60, 61] or the conical micro-modulus [36], which are used in this chapter. The CG solver is the most time-consuming part in the overall fatigue simulation because it requires solving the system produced by discretizing Eq. (3.10) at every point in a grid covering the domain, for every fictitious time step, until convergence is reached. Running the fatigue code on a single processor, the Intel Fortran profiler shows that more than 95% of the computational time is spent on the internal force calculation. To accelerate the numerical
simulations, in this chapter we use OpenACC directives (shown in Algorithm 2) on the serial code, to run internal force calculation on CUDA-enabled GPU devices. Minimizing the data transfer between CPU memory and GPU memory is a top priority while using GPU parallelized code. To save data transfer time, data which remain constant in the CG loop, like nodal displacements on boundaries, neighbor lists, etc., are sent to GPU memory beforehand and reside in GPU memory through all fatigue simulations. Before each GPU parallelized internal force calculation, new trial nodal displacements are transferred to the GPU memory. After internal force calculation on GPU, only the force density, and strain energy density are transferred back to CPU memory. To compare the GPU-enabled code and serial code, a static solution of a modified compact tension test is performed on a computer with Intel Xeon CPU E5-2630 and NVIDIA Tesla K20 GPU. Note that same convergence criterion and tolerance (see details in [36]) are used for computation on both CPU and GPU.

**Algorithm 1** The internal force routine for a linear peridynamic solid

```
!$acc kernels
for i ← 1, n do
    for j ← 1, n_fam do
        ξx = xi - xj; ξy = yi - yj; ξ = √(ξx^2 + ξy^2);
        ηx = ξx + duj - dui; ηy = ξy + dvj - dvi; η = √(ηx^2 + ηy^2)
        s = (η - ξ) / ξ;
        dfx = csVjηx/η; dfy = csVjηy/η;
        dw = cs^2 / 2ξ;
        f_x(i) = f_y(i) + dfx; f_y(i) = f_y(i) + dfy; w(i) = w(i) + dw

!$acc end kernels
```

Table 3.1 lists the computational time of solving a peridynamic static problems with three different horizon sizes on CPU and GPU-enabled code. Details of the simulated problems, including geometry, loading, and mesh are given in next section. Note that before performing the CG calculations, a peridynamic simulation needs to prepare necessary data, like searching neighbors for all nodes and/or correcting micro-modulus for nodes near the surface [66]. Time spent on this preparation are not included in the performance comparison in the table. The
CPU code has two versions, a scalar-based form shown in Algorithm 1, and a vectorized form, a conventional way for code optimization running on CPU (see pseudo code in Algorithm 2. Comparing the running times and speed-up factors, we can see:

- vectorized code on CPU is faster than the CPU code with nested loops, and getting faster as number of nodes increases.

- CUDA accelerated code on GPU is significantly faster than both versions of CPU code.

The performance advantage gained from GPU parallelization over the serial CPU code with nested loop is relatively constant with problem size.

<table>
<thead>
<tr>
<th>Node number</th>
<th>15155</th>
<th>34374</th>
<th>60562</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU (nested loops) time</td>
<td>57.9 s</td>
<td>268.4 s</td>
<td>671.6 s</td>
</tr>
<tr>
<td>CPU (vectorization) time</td>
<td>49.1 s</td>
<td>175.5 s</td>
<td>436.2 s</td>
</tr>
<tr>
<td>GPU time</td>
<td>2.9 s</td>
<td>11.7 s</td>
<td>35.0 s</td>
</tr>
<tr>
<td>CPU (nested loops)/ GPU</td>
<td>19.7</td>
<td>22.9</td>
<td>19.2</td>
</tr>
<tr>
<td>CPU (vectorization)/ GPU</td>
<td>16.9</td>
<td>15.0</td>
<td>12.5</td>
</tr>
</tbody>
</table>

Table 3.1: Computational time comparison between serial CPU code and GPU code

**Algorithm 2** Internal force routine for a linear peridynamic solid; vector (or matrix) operations follow the Fortran 90 syntax.

```plaintext
for i ← 1, n do ▷ loop through all nodes
    \( \xi_x(:,i) = X(:,i) - x_i \); \( \xi_y(:,i) = Y(:,i) - y_i \)
    \( \eta_x(:,i) = \xi_x(:,i) + U_x(:,i) - ux_i \); \( \eta_y(:,i) = \xi_y(:,i) + U_y(:,i) - uy_i \)
    \( \xi = \sqrt{\xi_x^2 + \xi_y^2}; \eta = \sqrt{\eta_x^2 + \eta_y^2}; \)
    \( S = (1 - D) (\eta - \xi) / \xi \) ▷ bond stain, \( D \) is damage flag
    \( dF_x = cSV \xi_x / \xi \); \( dF_y = cSV \xi_y / \xi \) ▷ periforce
    \( dW = cS^2 / 2 \xi \) ▷ strain energy density
for i ← 1, n do
    \( f_x = sum(dF_x(:,i)) \); \( f_y = sum(dF_y(:,i)); \)
    \( w = sum(dW(:,i)) \)
```

The performance gain by using OpenACC on GPU for a complete fatigue simulation are, obviously, smaller because here only the internal force calculation part is executed on the
GPU and repeated data transfers cut into the overall efficiency. For a fatigue simulation with 60562 nodes, the GPU code takes 7,045 s (about 1.96 hours), which is 5.03 faster than the vectorized CPU code of the same problem (35,443 s, about 9.98 hours). Compared with the serial code, the GPU code is 5.67 times faster (39,952 s, about 11.1 hours).

Another issue that needs attention is the memory usage on GPU due to their relatively limited memory. We estimate the memory usage on GPU based on parameters in the pseudo-code shown in Algorithm 2. We need to store the node family list, displacement, position, internal force, and strain energy density for every node (all in double precision floating-point arrays), and we also need a logical array to store bonds break information. Overall, for 2D problems with a ratio between the horizon size and grid spacing $\frac{\Delta}{\Delta x} = 4$, we need $605 \times n$ (where $n$ is the total number of nodes) bytes GPU memory to store all this data. Thus, the simulation with 60,562 nodes only requires about 37 MB GPU memory. With the NVIDIA Tesla K20 (5 GB GPU memory), we estimate we can run 2D peridynamic fatigue simulations or static analyses with about 8.0 to 8.5 million nodes. The speed up over CPU code obtained with minimal effort and modification of the serial code show that the performance advantages gained from using GPUs is very promising in modeling of fatigue fracture with peridynamics.

### 3.3 Simulation of crack propagation and validation against experiments

The peridynamic fatigue model is implemented in a Fortran code EMUNE. To validate the 2D peridynamic model for fatigue cracking presented in the previous sections, we adopt the configuration chosen in the experiments in [64]. The authors of [64], modified some compact tension (CT) specimens by adding circular cut-offs at various locations. By changing the position of the additional hole, the fatigue crack path changes direction significantly, and either ends up at the added hole, or moves slightly towards but bypasses it.
Figure 3.9: Geometry of the modified CT specimens (in mm) used in the experiments in [64]. The sample thickness is 8 mm.

3.3.1 Setups for modified CT tests

In the experimental work [64], the specimens are made from cold rolled SAE 1020 steel with Young’s modulus $E = 205$ GPa and Poisson’s ratio $\nu = 0.29$. All specimens were tested under at 20 Hz frequency with loading ratio $R = 0.1$. The crack growth rate was fitted to the following formula (see [64]):

$$\frac{da}{dN} = 4.5 \times 10^{-10}(\Delta K - \Delta K_{th})^{m},$$

(3.19)

where $\Delta K_{th} = 11.6$ MPa$\sqrt{m}$ is the threshold stress-intensity range below which the crack growth rate is negligible. In these experiments, loads were adjusted to maintain $\Delta K_1 \approx 20$ MPa $\sqrt{m}$.

To simplify the computational model preparation and coding, an uniform mesh ($\Delta x = \Delta y$) is used in the 2D peridynamic simulations of the samples seen in Fig. 3.21. After a $\delta$–convergence study (see next section), a value of 0.60 mm is adopted as the peridynamic horizon size, and the node spacing is $\Delta x = 0.15$ mm. This leads to a discretization with about 60,000 nodes. Note that in some peridynamic implementations, nodes on surfaces may
have half or quarter areas as nodes in the bulk (see, e.g., [59, 19, 60]), while in this chapter all nodes have same area (see also Fig. 3 in [66]). The uniform grid is arranged so that the pre-crack in the sample (see Fig. 3.21) separates nodes symmetrically.

We apply the so-called “volume correction” method that modifies the micromodulus of bonds near the boundary (including pre-crack surfaces) to reduce the well-known surface effect in peridynamics (see [66]). For example, the corrected micromodulus for a bond which connects nodes $x$ and its family member $\hat{x}$ is:

$$c_{\text{corrected}} = \frac{2V_0}{V(x) + V(\hat{x})}c$$

where $c$ is the micromodulus for nodes in the bulk computed based on Eq. (2.6), $V_0$ is the volume (area for 2D case) of the horizon region for a node in the bulk, $V(x)$ and $V(\hat{x})$ are volumes of the horizon regions of nodes $x$ and $\hat{x}$, respectively. For a detailed discussion of various surface correction methods please see [66].

All simulations start with an initial crack (along the $x$-axis of our coordinate system) of length 0.9 mm, at the tip of the pre-notch shown in Fig. 3.21, same as in experiments. Force density, equivalent to force $P$ (see Fig. 3.21), is applied only on the nodes with maximal absolute value of vertical position on the boundaries of two pin holes. This loading method ignores the variation of force in experiments where specimens, loaded through pins, are allowed to rotate [67]. Our simulation results match well with experiments, which indicates that the influence of force variation is minimal.

To maintain the effective stress-intensity range $\Delta K_1$ at the 20 MPa$\sqrt{m}$ level as in experiments, the SIF is calculated based on the J-integral (see Section 3.2.2) and then used to update the magnitude of $P$ as follows: in the first iteration, a load $P=6$ kN produces $\Delta K_1$
close to 20 MPa$\sqrt{\text{m}}$; for all other iterations, the magnitude of loading is updated by:

$$P_n = P_{n-1} \Delta K_I / \Delta K_n$$

where $\Delta K_n$ is calculated using Eq. (3.18). Note that, due to the asymmetry of the sample caused by the added hole, the J-integral value contains some small mode II contribution. This may result in a slightly higher magnitude of loading $P$ than required in pure mode I to achieve $\Delta K_I = 20 \text{ MPa } \sqrt{\text{m}}$. These tests are mode I dominated and we expect the influence of larger loading magnitude on the results to be minimal.

### 3.3.2 Convergence studies for crack path and fatigue life

Three types of numerical convergence in peridynamic simulations were proposed in [50]. The $m$-convergence, in which the spatial integration accuracy is increased (for a fixed horizon size), was discussed for 2D fracture problems in isotropic materials [18, 19], and $\delta / \Delta x = 4$ is chosen in the present work. Here, we focus on $\delta$-convergence, which uses a fixed horizon factor $m = \delta / \Delta x$ and decreases the horizon size. The CT1 sample is used in the convergence study, with three different grids densities corresponding to three different horizon sizes: 2.4, 1.2, and 0.6 mm, respectively. These horizons are about 68%, 34%, and 17% of the radius of the added hole, $r_{\text{hole}}$, respectively. The corresponding number of nodes are about: 4,000; 15,000; 60,000. The parameter $p_2$ is 2.1, according the crack growth rate function from
experiments [64]. We compute parameter $A_2$ using Eq. (3.9) and find $A_2 = 1.73e7$, $9.53e6$, and $8.97e6$ for $\delta = 2.4$, $1.2$, and $0.6$ mm, respectively.

In Fig. 3.11 we compare the measured experimental crack path of CT1 test and the peridynamic results with the three different horizon sizes. The experimental result is extracted from Fig. 16 in [64]. The peridynamic crack paths (see Fig. 3.10) have a “thickness” of $2\delta$ (in bond-based PD, see [18]) and crack paths are represented by partially or fully damaged nodes, with damage factors $0 < d < 1$. To simplify data processing, we convert damage maps produced by the PD simulations to black and white images in Matlab. Then we use thinning operation (using the `bwmorph` function with “thin” option in Matlab) to reduce crack paths to single pixel thickness, and find endpoints of crack paths to get crack tips (using the `bwmorph` function with “endpoints” option in Matlab). For example, crack tips and crack paths for a modified compact tension test are extracted in Fig. 3.12.

With the least number of nodes and the largest horizon size ($\delta = 0.68r_{hole}$), the crack sinks in the hole. After decreasing the horizon size to $0.34r_{hole}$, the simulated crack path avoids the hole and is similar to that from experiments. With the further decrease of horizon size, only small changes in the crack path happen and the computed paths get closer to the
Figure 3.12: Morphological operation with Matlab to extract crack tips and crack paths of simulation results, red dots are crack tips found by Matlab code.

experimental one. We conclude that convergence of crack path is achieved, considering that the crack paths are close to that seen in experiments and results obtained with the two smaller horizons ($\delta = 0.34r_{\text{hole}}$, and $0.17r_{\text{hole}}$) are almost the same.

Fig. 3.13 shows the fatigue life comparison between experiment and peridynamic simulations. A slightly curved fatigue life is obtained in the experiments (see [64]) although the experimentalists tried to maintain a constant $\Delta K_I$ and a constant crack growth rate $da/dN$. In contrast, the PD results show a linear fatigue life since we enforce constant values for these quantities. The slopes of the fatigue life curves given by the PD results with the three different horizons are almost identical. The result for $\delta = 2.4$ mm is a shorter line because the crack path for this case is different.

In section 3.3.4, we will obtain better agreement with the experimental fatigue life since we use different $A_2$ values in different cycle ranges, mimicking actual conditions in the experiment. Through the convergence study in terms of crack path and fatigue life predictions, we can conclude that $\delta = 0.6$ mm provides results that match well with experiments. For the remaining of this chapter we use this horizon size (and a horizon factor $m = 4$).
3.3.3 Crack-path predictions

As observed in the experiments in [64], the fatigue crack path is sensitive to the position of the added hole. By slightly changing the position of this hole, two types of fatigue crack paths are obtained: missing the hole or sinking in the hole. These two crack growth patterns are successfully predicted by the peridynamic fatigue crack model, as shown in Fig. 3.14.
For all specimens, simulated crack paths are extracted from damage maps (see Fig. 3.14) and compared with data from Fig. 16 in [64]. In the PD results, all cracks start growing from same location, the tip of the pre-crack (see Figs. 3.14 and 3.15). The black curves, which are the experimental results extracted from [64], should contain the pre-crack section for all specimens, because these curves are extracted from sample images. However, the experimental results in [64] are a little unclear on this point. For example, for CT4 the straight pre-crack portion is apparently missing. This could be due to the way in which the pre-crack was prepared, as they mention in their paper. Because of this, in the 3D sample one may end up with slight differences between the fatigue crack paths on the front and back side of the sample. This could explain the differences between simulated results (PD and the FEM-based from [64]) and the experiments seen for the CT4 test.

We see that, for CT1 and CT2 tests, the PD results match very well the observe crack path even when the FEM-based results from [64] start to depart from the experimental results.

Assuming that CT4 experimental test was conducted in the absence of a pre-crack, we perform a PD computation for CT4 without a pre-crack. The crack paths are compared in Fig. 3.16. The PD result without a pre-crack now matches closer to the experimental path, but it starts to separate from it at about the mid-point of the total length. This, again, could be due to sample imperfections and 3D deformation effects (existence of transversal moments). The authors of [64] do mention that they noticed slightly different crack paths on the two sides of the sample. For samples CT3 and CT4, they show different life prediction curves for the two sides of the samples (see Fig. 3.17).

3.3.4 Fatigue life predictions

In the convergence study in section 3.3.2, the crack growth rate is obtained as linear. The crack growth rate was $da/dN = 8.97\times10^6$, based on Eq. (3.19) with $p_2 = 2.1$. In the experiments
Figure 3.15: Crack paths for different CT specimens comparing experimental and FEM results from [64] with our peridynamic results.
Figure 3.16: Crack paths for CT4: one of the PD solutions assumes no pre-crack, and the experimental path from [64] seems to be obtained without a pre-crack also.

in [64], while the loads were adjusted in order to maintain and approximately constant $\Delta K_I$, the resulting crack growth rate is slightly nonlinear (see Fig. 3.13). In order to match with our PD simulations this measured, variable, crack growth rate, we use different $A_2$ values over different cycle ranges. Table 3.2 lists the values for $A_2$ used for simulations of the CT1 to CT4 tests. For example, the values for $da/dN$ are obtained for the CT1 case by using the experimental data from Fig. 3.17: over the cycle number range $N < 0.19 \times 10^6$, we extract $da/dN = 3.25 \times 10^{-9}$, while for the cycle number range $N \geq 0.19 \times 10^6$ we extract $da/dN = 4.62 \times 10^{-9}$. These lead to the values for $A_2$ shown in the first column of Table 3.2.

With these modification, the fatigue lives from the PD results match well with the experimental data (see Fig. 3.17). As mentioned before, in the experiments with the CT3 and CT4 samples, different crack paths are obtained on the two side of the sample (see Fig. 3.17, bottom two figures). The FE results given in [64] aim to match the averaged experimental results. FE fatigue life for CT3 is closer to data of side 2, and FE results for CT4 matches well except that the final region of simulated fatigue life is much lower than seen in experiments. For the peridynamic fatigue simulations, we choose to calibrate the parameters in table 3.2 to experimental data of side 1 for CT3 and CT4. Good match with experiments is observed.
Figure 3.17: Fatigue life predictions: comparisons between our peridynamic results and experimental and FEM-based simulations from [64].
Table 3.2: Values of $A_2$ used in the PD simulations for different cycle ranges and different sample types ($\tilde{N}$ is cycle number divided by $10^6$).

<table>
<thead>
<tr>
<th>CT1</th>
<th>CT2</th>
<th>CT3</th>
<th>CT4</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.71e6, $\tilde{N}&lt;0.19$</td>
<td>6.98e6, $\tilde{N}&lt;0.26$</td>
<td>9.13e6, $\tilde{N}&lt;0.06$</td>
<td>1.29e7, $\tilde{N}&lt;0.06$</td>
</tr>
<tr>
<td>1.10e7, $\tilde{N}\geq 0.19$</td>
<td>6.27e6, $\tilde{N}\geq 0.26$</td>
<td>1.65e7, $0.06\leq\tilde{N}&lt;0.12$</td>
<td>8.06e6, $0.06\leq\tilde{N}&lt;0.08$</td>
</tr>
<tr>
<td>1.41e7, $\tilde{N}\geq 0.12$</td>
<td>1.65e7, $0.06\leq\tilde{N}&lt;0.12$</td>
<td>1.84e7, $0.08\leq\tilde{N}&lt;0.12$</td>
<td>6.02e6, $\tilde{N}\geq 0.12$</td>
</tr>
</tbody>
</table>

3.4 Fatigue cracks of a two-phase composite

In this section, fatigue damage of a two-phases composite is performed to highlight the advantages of peridynamic fatigue simulations in terms of multiple crack growth and crack interactions compared with other methods. The two-phase composite model (see Fig. 3.18) is from a digitized scanning electron microscopy (SEM) image of superconducting filaments (Bi2201) embedded in a silver matrix (see [54]). Stress analysis and strength of this material are investigated with peridynamics in [54]. The original SEM image is 1113 by 816 pixels, and each pixel is about 0.14 $\mu$m.

Table 3.3: Material properties of Bi2201 and silver

<table>
<thead>
<tr>
<th>Young’s modulus (GPa)</th>
<th>Poisson ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silver</td>
<td>91.0</td>
</tr>
<tr>
<td>Bi2201</td>
<td>39.4</td>
</tr>
</tbody>
</table>

We choose a horizon size $\delta = 5.6\mu$m and a uniform grid with about 10,000 nodes, having node spacing equal to 1.4 $\mu$m. A force density equivalent to 10 MPa pressure is applied on a single layer of nodes on the left and right boundaries to set the sample in tension. Just for demonstration purposes, to enhance the number of fatigue-cracks initiation points and the number of crack interactions, a region of thickness $\delta$ is assigned as a “no-fail” zone on the
Figure 3.18: Image use to generate peridynamic model for two-phase composite, the white region are silver and black region is superconducting filaments. A black frame used to show the boundary of the sample left and right boundaries. Elastic material properties for this two-phase material are listed in Table 3.3.

The sample is intact at the beginning. All three phases of fatigue are used in this simulation: fatigue crack initiation, growth, and final failure. As introduced by Silling in [29], phase I will transfer to phase II once a node and/or a node within its horizon has a damage index larger than 0.5. The transition from phase II to phase III is shown in the flowchart given in Fig. 3.3. Two assumptions are used in the fatigue for this composite material simulation:

- The two material components use the same group of fatigue parameters (because this example is for illustration purpose only);

- The interface between the two material components is easier to break than either of the components by setting the initial remaining life of peridynamic bonds crossing a material interface to be half of other bonds.

Snapshots of the evolution of damage at 8000, 14000, 20000, and 22000 cycles are shown in Fig. 3.19. Four crack initiation sites can be seen in Fig. 3.19a, including two caused by material discontinuities and two near the boundaries where the loading is applied. In Fig. 3.19b we see that new cracks initiate and growth along the interface of the two materials and within the superconducting filaments. Complex crack interactions, like crack coalescence, can be observed in Fig. 3.19c. Final failure occurs as shown in Fig. 3.19d. We emphasize that
Figure 3.19: Snapshots of damage results of the two phases material

this simulation was obtained with the same model used in the homogeneous and isotropic sample in the previous sections. The only difference is in the input data that defines the material properties at a node. This example shows that the peridynamic fatigue model can be used to simulate complex fatigue crack initiation, growth and final failure in composite materials.
3.5 Modeling all three phases of fatigue failure with peridynamics

In the original peridynamic fatigue model [29], the crack propagation phase is calibrated to Paris’ law data. However, this model ignored the fact that the Paris’ law is not valid when the stress intensity range is smaller than its threshold. We observe that ignoring the threshold, the remaining life of bonds continues to decrease around developed crack paths, independent on whether the threshold is met or not. We explain this issue by simulating a modified compact tension test. Results indicate that the original model leads to the fatigue crack sinking into the hole, as expected, but when simulations are continued, instead of a new crack being initiated somewhere on the other side of the hole, damage forms around the original crack and an unphysical fatigue crack path is obtained instead. We extend the model to incorporate a “fatigue limit”, calculated based on the threshold stress intensity range, in the crack propagation phase. We provide convergence results for crack paths and fatigue lives, under reducing the size of the nonlocal region (and refining, correspondingly, the grid spacing), for a relatively complex fatigue crack growth scenario. Crack paths agree with the strain concentrations produced by quasi-static elastic analysis. The peridynamic model for fatigue fracture is able to continue the simulations through full failure of the sample, and we observe the expected large rotations of the sample past final failure. The results demonstrate the effectiveness of the proposed extension in modeling of complex fatigue crack growth.

3.5.1 An extension of the peridynamic fatigue model

The fatigue limit is the amplitude of cyclic stress below which the material can be cycled for either an infinite or a sufficient number of cycles without fracture [68]. In [29], the evolution law of remaining life is

\[ \frac{d\lambda}{dN}(N) = -A\varepsilon^p, \]  

(3.21)
and the fatigue limit is incorporated in the crack initiation phase by modifying the evolution law of remaining life as follows:

\[
\frac{d\lambda(N)}{dN} = \begin{cases} 
-A_1(\epsilon - \epsilon_\infty)^{p_1}, & \text{if } \epsilon > \epsilon_\infty, \\
0, & \text{otherwise.}
\end{cases}
\] (3.22)

In this equation, \(\epsilon_\infty\) is the fatigue limit, expressed in terms of strains, for the crack initiation phase. Numerical examples in the remaining sections show the implementation details of phase I model with this fatigue limit.

As discussed above, the phase II of this peridynamic fatigue model is calibrated by matching with experimental Paris’ law, which relates the range of stress intensity factor and the crack propagation rate. Because the crack ceases to advance if the stress intensity range is smaller than a threshold value \(\Delta K_{th}\) \cite{69}, we introduce an extension of the model to incorporate the threshold stress-intensity range. Similar to Eq. (3.22), we can modify the crack propagation law in Eq. (3.21) by adding a fatigue limit \(\epsilon_\infty\) for the crack propagation phase, as follows:

\[
\frac{d\lambda(N)}{dN} = \begin{cases} 
-A_2\bar{\epsilon}^{p_2}, & \text{if } \epsilon > \epsilon_\infty, \\
0, & \text{otherwise.}
\end{cases}
\] (3.23)

Because the range of stress intensity is proportional to the strain, \(\epsilon_\infty\) can be calculated based on the following equation:

\[
\frac{d\lambda(N)}{dN} = \begin{cases} 
\epsilon_\infty \bar{\epsilon}, & \text{if } \Delta K_{th}, \\
0, & \text{otherwise.}
\end{cases}
\] (3.24)

in which \(\bar{\epsilon}\) is the average cyclic strain of bonds connected to the crack tip. In this way, the remaining life \(\lambda\) is "frozen" if \(\Delta K < \Delta K_{th}\). This prevents unphysical fatigue crack propagation. To accomplish this step, here we do not need to track the crack tip.
Table 3.4: Calibrated peridynamic fatigue model parameter for SAE 1020 steel

<table>
<thead>
<tr>
<th>Phase</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>$A_1$</td>
<td>1.32e15</td>
</tr>
<tr>
<td></td>
<td>$p_1$</td>
<td>9.0</td>
</tr>
<tr>
<td></td>
<td>$\epsilon_{\infty}$</td>
<td>0.001</td>
</tr>
<tr>
<td>II</td>
<td>$A_2$</td>
<td>7.76e6</td>
</tr>
<tr>
<td></td>
<td>$p_2$</td>
<td>2.1</td>
</tr>
<tr>
<td></td>
<td>$\epsilon_{\infty}$</td>
<td>0.0001</td>
</tr>
</tbody>
</table>

Algorithm that tracks the crack tips of any number of cracks, based on Matlab’s image processing functions, please see [36]. Once the crack tip location is determined, we compute the peridynamic J-integral on a contour surrounding it, as discussed in [36]. This chapter until a crack sinks into an existing perforation, hole, or defect, when the contour may need to be modified so that it surrounds such holes or defects as well. We then compute the stress-intensity range and compare with the threshold value to decide whether we modify the remaining life or not.

3.5.2 Calibration of numerical parameters to experimental data

In this section, we focus on the parameter calibration for phase I with fatigue limit, and for phase II considering the stress intensity range. Table 3.4 shows values of calibrated parameters used in phase I and phase II for SAE 1020 steel. In phase I, the peridynamic model is set to match S-N data from [22]. The fatigue limit, in terms of strains, is 0.001 based on experimental data [23]. The calibration method is provided in [12]. Redrawing the S-N curve in a log-log plot, the slope of S-N curve is $-1/p_1$, and the intersection with Y-axis is $-\log A_1/p_1$ (see Fig. 3.20).

For phase II, the $p_2$ value can be obtained from the fitted Eq. (3.26) in [64]. To determine $A_2$, since $\beta$ in Eq. (3.7) is not known in closed form, we need to find an alternative route. We can perform a single peridynamic simulation of fatigue crack growth with an arbitrary
value of $A$ and the calibrated value. The simulation will provide a certain crack growth rate $da/dN$. Because the crack growth rate depends linearly on $A_2$, the $A_2$ which can produce experimental crack growth rate can be calculated as:

$$A_2 = A \frac{da/dN}{da/dN}.$$  

(3.25)

To calculate the fatigue limit $\epsilon_\infty$ in phase II, we use Eq. (3.23) with $\Delta K_{th} = 11.6 MPa \sqrt{m}$ and $\Delta K = 20 MPa \sqrt{m}$.

Figure 3.20: The experimental SN curve, and peridynamic model results with and without the fatigue limit (experimental test data from [22]).

We now test the proposed model for a simple fatigue crack growth case. A standard compact tension (CT) test, in which a crack propagates in a self-similar way from an existing notch, was simulated in [29]. The original fatigue model has not been tested for problems in which the fatigue crack, for example, encounters a hole, and may continue from another location. Do perform such a test, we use a modified CT specimen with an additional hole, shown in Fig. 3.21. The fatigue crack propagates and sinks into the added hole. Fig. 3.22 show the damage results by original and extended peridynamic fatigue models. Both models, the original model and the one proposed here with the fatigue limit in phase II, produce the same result up to the point when the crack sinks into the hole. The results from the two
models, however, depart from each other once that crack reaches the hole: with the original model, “thickness” of the damage along the crack path continues to increase and, eventually, two new cracks nucleate from two corners of the geometry. This behavior is a result of:

- An algorithmic-related reason (lack of fatigue limit in phase II): in the original model, a node switches from phase I to phase II if a node within its horizon has damage index larger than 0.5. Bonds connected to nodes that are in phase II continue to have their remaining live decrease with cycle number as long as there is some nonzero strain at those locations.

- A geometric-related reason: the small strain concentration at two corners of the specimen, coupled with the evolution law for the remaining live of bonds near these regions, leads to crack growth from regions not normally expected to show fatigue cracks.

![Figure 3.21: Geometry of the modified CT specimen (dimensions are in mm)](image)

In contrast, the new, extended model, shows a new crack nucleating on the left side of the added hole, as expected. This result agrees with the quasi-static strain analysis: the region with highest strain concentration shifts from the crack tip to the left boundary of the hole, once the crack sinks into it.
3.5.3 Model validation for a modified compact tension test

In this section we validate our model against some known experimental results for modified compact tension test with an asymmetrically positioned added hole. While experimental results are not available for the fatigue past the sinking of a crack into the hole, quasi-static analysis gives a good indication of how we might expect the fatigue failure to proceed past that stage. We will see again that, without considering the threshold for the crack propagation phase, the peridynamic fatigue model produces unexpected fatigue crack paths for the stage following the sinking of the first crack into the added hole of the modified CT specimen.

In Fig. 3.23 we give the geometry of a modified compact tension (CT) tests by Miranda et al. [64]. The specimen has two pin holes used to apply the loading and one cut-off ahead of the crack tip, positioned asymmetrically relative to the horizontal symmetry line of the sample.

The specimen is made of cold rolled SAE 1020 steel with Young’s modulus $E = 205 \text{ GPa}$ and Poisson’s ratio $\nu = 0.29$. All specimens were tested, in the experiments in [64], at 20 Hz frequency with loading ratio $R = 0.1$. The initial crack is 0.9 mm. The crack growth rate
was fitted to formula:

\[
\frac{da}{dN} = 4.5 \times 10^{-10}(\Delta K - \Delta K_{th})^{2.1},
\]

(3.26)

where \(\Delta K_{th} = 11.6 \text{MPa} \sqrt{\text{m}}\) was the threshold stress intensity range below which crack growth rate is negligible. In the experimental work, loads were adjusted to maintain \(\Delta K \approx 20 \text{MPa} \sqrt{\text{m}}\).

In the experimental results in [64], the fatigue crack path changes direction significantly depending on the position of the added hole. The crack path either ends up at the hole (for CT2 and CT4 samples, see Fig. 3.23), or moves slightly towards but bypasses it (for CT1 and CT3 cases). The crack growth behavior and fatigue lives are accurately captured by the peridynamic fatigue cracking model (see [36]). Here we want to see what happens, computationally, after the crack sinks into the hole, and for this reason we only simulate the fatigue crack growth for the CT4 geometry.

Figure 3.23: Geometry of the modified CT specimen (dimensions are in mm) used in the experiments in [64]. The sample thickness is 8 mm.

To perform the peridynamic simulations, we use a 2D plane strain model with a uniform mesh. We are interested in the convergence behavior in terms of the horizon size, to answer the question: what happens to the fatigue crack paths when the horizon is reduced?

We use three different horizon sizes (1.2, 0.8, and 0.6 mm; notice that the hole size
diameter is 7 mm)) and three different grids corresponding to these horizons, so that the same horizon size factor ($\delta/\Delta x=4$) is achieved. The corresponding number of nodes in these grids are: 15,155; 34,374; 60,562. For simplicity, we apply concentrated loads as shown by two red arrows in Fig. 3.23. This is different from the distributed load application in the experiments, but it should not influence our results. Because of the concentrated applied loadings, however, we need to assign "no-fail" zones around the loading holes to prevent damage initiation at these locations. Therefore, a $2\delta$ thickness annulus shaped no-fail region (shown by dashed line in Fig. 3.23) is assigned around the two pin holes.

Fig. 3.24 shows the crack path from the experiment at about cycle $N = 130,000$. At this cycle number, the simulated crack paths by the peridynamic model (the existing or the extended one) with three different horizon sizes (and three different discretizations) agree very well with the experiment.

![Figure 3.24: Crack paths of experimental work (left-most, from [64]) and peridynamic simulations (existing or extended model) with three different horizon sizes (left to right in decreasing order of horizon size used). All results are shown at cycle number 130,000.](image)

We let the simulation run beyond the experiments, to investigate the fatigue behavior after the crack sinks into the hole. Fig. 3.25 shows the damage map and strain energy plot after the crack sinks into the added hole. We note that, up to this point, the same results if obtained by the existing peridynamic model or the extended one. Once the crack sinks in the hole, strain concentrates at:
• The two points where loadings are applied (shown by red arrows in Fig. 3.25);

• The crescent-shaped region on the left side of the added hole.

Based on the strain concentration results and the no-fail zone imposed around the two pin holes, we expect a fatigue crack to nucleate around the added hole within the strain concentration region.

Observe that, once the crack reaches the hole, the structure’s compliance changes dramatically and maintaining the same $\Delta K$ as before (and as in experiments) is not sufficient to create a new fatigue crack growth. To investigate fatigue crack growth or damage after the crack sinks in the added hole, we increase (by 0.5% percent after every 300 fictitious time steps) the loading magnitude, as well as the strain limit in Phase II proportionally, until new bonds start to break again. Once the initiation of a new crack happens, we maintain a constant loading magnitude until the end of the simulation.

In [36], the algorithm used goes back half a step when too many bonds break from one iteration to the next, to prevent numerical instabilities. In this thesis, an adaptive approach is used to determine the new fictitious-time step size when too many bonds break in one iteration. This is based on the critical damage index proposed in [36], which measures the largest difference between nodal damage index at all nodes in the domain; when this difference is larger than a preset value, then we back-track and use half the time step. The halving procedure continues until the criterion for critical damage index parameter is satisfied. Without this backtracking approach in determining the appropriate fictitious time-step, numerical instabilities can lead to non-physical cracks being initiated in multiple locations. This is especially important for problems in which crack nucleation happen from a wide strain concentration region, as in the case shown in Fig. 3.24.

Fig. 3.26 shows the damage index map with the original peridynamic fatigue model. After the crack sinks in the hole, as expected, a new unexpected crack develops from the
original crack path and propagates toward the left boundary. The reasons for this behavior are similar to those mentioned in the previous section: the remaining life for bonds on the crack surface continues to decrease because the strains around the crack that sank into the hole are small, they are not zero. The applied loads are not sufficient to initiate a new crack at the high strain spot on the left side of the hole, but they are large enough to create small strain concentrations at the place where the crack turns towards the hole. Without the limiting value of the threshold stress intensity range, a new crack starts propagating from the existing fatigue crack.

With the extended model, a new crack nucleates from the left side of the added hole after the original crack sinks into it. Fig. 5.14 shows nucleated cracks using three different horizon
sizes (and their corresponding computational grids mentioned before). To demonstrate the further advantages of the extended peridynamic fatigue model, we let the nucleated cracks propagate until final failure, thus activating the third phase of fatigue failure: quasi-static fracture caused by bonds reaching their critical bond strain value. Because the experiments in [64] do not cover this portion of fatigue failure, we only focus on the overall, expected behavior of failure.

![Figure 3.27](image)

Figure 3.27: Crack nucleation after the original crack sinks into the added hole. Damage maps obtained with the three different horizon sizes and their corresponding grids. From left to right: $\delta = 1.2$, 0.8, and 0.6 mm, respectively.

Figs. 3.28, 3.29, and 3.30 show, for different horizon sizes, the evolution of cracks propagation and final failure in the specimen from the moment the second crack approaches the edge of the sample, through full sample failure. The snap-shots are taken at the same cycle numbers for each of the solutions. The convergence of the crack path with smaller and smaller horizon sizes becomes clear from studying these figures. Results show that the second nucleated cracks propagate (almost horizontally) toward the left boundary of the specimen in phase II. The switch to fatigue phase III is automatic, once the crack tip approaches the edge. We can see the final failure of specimens, which break into two parts, as the result of phase III failure.

With the improved model provided in this chapter, we demonstrate a major advantage of the peridynamic fatigue model: simulation of three phases of fatigue failure. In particular,
the extension makes the fatigue model capable of simulating new cracks initiation and propagation after original cracks sink into holes.

![Figure 3.28](image1.png)

Figure 3.28: Damage index map showing the transition between fatigue crack growth and quasi-static fracture/final sample failure. Results obtained with horizon size 1.2 mm.

![Figure 3.29](image2.png)

Figure 3.29: Damage index map showing the transition between fatigue crack growth and quasi-static fracture/final sample failure. Results obtained with horizon size 0.8 mm. Snap-shots taken at the same times as in Fig. 3.28.

The new model requires the computation of the stress-intensity range at every fictitious-time step to determine whether its value is above the threshold value or not and adjust, or not,
Figure 3.30: Damage index map showing the transition between fatigue crack growth and quasi-static fracture/final sample failure. Results obtained with horizon size 0.6 mm. Snap-shots taken at the same times as in Fig. 3.28.

The remaining life of bond in strain concentration regions. This calculation requires the computation of the peridynamic J-integral value, in our previous work, [36], this calculation was only needed for matching the way applied loads are controlled in experiments. In the new model, the crack tip needs to be tracked and the stress intensity range needs to be computed at all times, except for when the $\Delta K$ value is maintained constant, allowing us to calculate the fatigue limit at the tip of the pre-crack at the first time step only.

3.6 Conclusions

We extend a recently developed fatigue crack model based on peridynamics to improve computational efficiency and ensure numerical stability. We perform extensive simulations to validate the model against experimental results. We also provide an illustrative example of the three phases of fatigue (crack initiation, crack growth and interactions, and final failure) in modeling of fatigue cracking in a two-phase composite material with a complex
microstructure.

We simulate fatigue cracks for modified compact tension (CT) tests and the peridynamic results are compared with available experimental data in terms of crack path and fatigue life. We use a 2D model with plane strain assumptions to simulate the 3D samples used in experiments. We obtain the static solutions via energy minimization by the conjugate gradient solver and introduce a new set of damage factors in the algorithm for phase II of fatigue that: 1) ensures equilibrated configurations after breaking of bonds, and 2) results in efficient computations. Convergence studies are performed to determine these damage factors. We also perform convergence studies in terms of decreasing the horizon size. Results show that this model agrees well with experiments even for fairly coarse grids. To mimic experimental setup of CT tests, constant stress intensity factor is maintained by calculating the peridynamic J-integral.

By comparing with experimental data for the fatigue crack paths and fatigue lives, we conclude that the peridynamic fatigue crack model provides accurate prediction. Advantages of the peridynamic fatigue crack model are:

- No criteria are needed to guide the direction of crack growth. In FE or other methods, the crack growth direction is calculated based on criteria, like the maximum circumferential stress criterion. In the peridynamic model, cracks autonomously initiate and advance after bonds break. For any new crack behavior, like crack branching, new criteria are needed in other methods, however, the peridynamic fatigue model can simulate all of these behaviors without any modification.

- This peridynamic fatigue crack model can be used to simulate multiple cracks growth, coalescence and diffuse damage evolution, without any extra criteria, normally needed in other approaches.

An extension is proposed to improve a recently developed fatigue crack model based on
peridynamics. The crack propagation phase in the original model was calibrated with Paris’ law but the model ignored to take into account the threshold value of the stress intensity range, which prevents growth if the applied loads create a stress intensity below a certain value. Because of that, once a crack sinks into a hole, for example, the fatigue crack path evolves in unexpected ways with the original model. We have explained the reasons behind the puzzling behavior and have introduced the threshold value into the new model. The modified model produces fatigue crack paths that are consistent with expectations, even when geometrical features, like holes, are encountered by the propagating fatigue crack.

We have performed convergence studies in terms of the fatigue crack path and fatigue life by using three different horizon sizes (all sufficiently smaller than the size of the hole in the modified CT specimen) and their corresponding computational grids, setup so that the ratio between the nonlocal region size and the grid spacing was the same for all calculations. Our simulation results show that the model is able to predict the three phases of fatigue failure: fatigue nucleation, propagation and final failure, in a relatively complex failure scenario in which a fatigue crack sinks into a hole before continuing, under modified loading conditions, to initiate and propagate from a new location through final failure.

We also proposed a very simple way for accelerating peridynamic fatigue crack growth computations by sending the internal force calculations to the GPU. The speed up over the serial CPU code, and the minimal effort required in modifying a serial code for this purpose, are remarkable.
Chapter 4 Dynamic brittle fracture of AlON

One of the main mechanisms through which ceramic materials fail under mechanical loading is brittle fracture. In order to predict the performance and structural integrity of such materials, a fundamental understanding of brittle fracture in polycrystalline ceramics at the grain-size level is required [70]. Such an understanding can then be used to design advanced structural ceramic systems with increased impact resistance, higher thermal shock resilience, etc. Here we present a novel approach for simulating fracture in polycrystalline ceramics, which has been difficult to do in the past, due, in no small measure, to the complexity of the phenomenon [71].

Combined transgranular (cracks pass through the grains) and intergranular (cracks propagate between the grains) fracture can happen in brittle fracture of ceramics [30]. A transition between trans- and inter-granular fracture is observed under certain conditions of loading rates when the crack starts running unstable. Experiments [72] show the dependence of fracture characteristics of silicon nitride ceramics on the existence of crystalline phase at triple junctions. While the observed main fracture mode is intergranular [72], local transgranular fracture also appears due, apparently, to the existence of crystalline phase at grain junctions. Also, crack deflection and crack bridging mechanisms were observed due to the presence of large, rod-like grains. Further evidence of the importance of accurate modeling of inter- and trans-granular fracture in polycrystalline ceramics investigated by a theoretical model of intragranular particle residual stress strengthening [73]. The SiC nanoparticles in the $Al_2O_3$ grains create a normal compressive stress at the grain boundaries and a tangential tensile stress in the grains, resulting in the “strengthening” of the grain boundaries and “weakening”
of the grains. Accordingly [73], there exists an optimum amount of SiC for strengthening, below which the grain boundaries are not fully “strengthened” and the fracture is mainly intergranular, above which the grains are “weakened” too much and the fracture is mainly transgranular, and at which the fracture is a mixture of intergranular and transgranular. Toughening mechanisms in nanocomposites are reviewed [74].

Existing models [31, 13] for simulating brittle fracture in polycrystalline ceramics that can include combined trans- and inter-granular crack propagation have severe limitations, including: the inability of modeling propagating cracks that naturally coalesce and/or branch; limitation to modeling only a single or just a couple of cracks; complicated algorithms that cannot extend to 3D, etc.

The FEM has been the preferred tool used in numerical models of polycrystalline materials [31, 75, 71, 76]. Fracture in polycrystalline materials has been modeled using cohesive-zone models [77, 78]. In recent years, cohesive surface models have been widely used to numerically simulate fracture initiation and growth by the finite-element method [13, 79, 80, 81]. Recently, some difficulties regarding time discontinuities in cohesive zone models have been pointed out [82], and bias of the crack propagation path [83]. Mathematical and physical limitations and constraints on cohesive laws have been pointed out [84].

In numerical modeling brittle fracture of polycrystalline ceramics, the most common approach is to consider only intergranular fracture: cracks are restricted to grain boundaries [85, 86, 71, 87, 88, 89]. Finite elements with a “soft-kill method” [76] are used to propagate the crack along grain boundaries instead of using a cohesive zone model.

Crack propagation behavior in alumina polycrystals has been analyzed [90] using the body force method (BFM) [91] which employs superposition of fundamental solutions. Combined trans- and inter-granular fracture is simulated, but the solutions are based on relations postulated for the mode I to mode II transition and an existing initial crack is postulated. More recently, a two-dimensional XFEM [92] with level sets model [93] for studying the
transition from intergranular to transgranular crack growth in polycrystalline materials has been proposed. It is not clear that this model can be extended to treating multiple cracks in fragmentation scenarios or dynamic problems in 3D.

Lattice spring models have been used to study brittle fracture and damage in polycrystalline materials [94, 95]. In the brittle spring network, a spring fails if the stored elastic energy in the spring exceeds a critical value. A transition from intergranular to transgranular fracture with increasing grain boundary toughness is observed [94], however, these studies are limited to 2D quasi-static analysis.

Compared to existing methods, the peridynamic model [1, 32] used here for analyzing crack initiation, propagation, and fragmentation in a rate-dependent mechanically loaded Voronoi polycrystalline ceramics has important advantages because:

- The cracks initiate and propagate when and where is it energetically favorable to do so [20];
- Inter- and transgranular fracture are direct consequences of the computations and they do not have to be postulated via ad hoc assumptions as is the case for the classical approach [33];
- Mode-transition and mode-mixing of crack propagation is naturally captured by the peridynamic formulation [18, 19, 21];
- Fracture at triple-junction points is not controlled by ad-hoc assumptions but by the actual loading conditions in the region surrounding the triple-junctions [33];
- Complex interaction between cracks does not have to be assumed, but rather it is part of the solution [21, 20];
- The meshfree character eliminates the need for complex meshing algorithms of Voronoi polycrystals.
Here we introduce a new bond-based PD model for 3D polycrystalline materials and use it to understand the supershear damage propagation in Edge-on Impact (EOI) on polycrystalline ceramics observed in the experiments reported in [30]. With the same average grain size as of the sample use in experiments, we create a scale-down version of the experiments that mimics the same impact-generated stress over an area on the edge of the sample. The results produced by the PD model clearly capture the evolution of damage on the sample surface reported in [30]. Moreover, we investigate damage evolution through the sample thickness, which is difficult or impossible to do in experiments. The obtained propagation speeds for the damage front and localized cracks springing from it match closely the values obtained experimentally.

4.1 Cubic elasticity

AlON is an anisotropic crystalline material with cubic spinel structure. Hooke’s law for the cubic crystal is

\[
\begin{bmatrix}
\sigma_1 \\
\sigma_2 \\
\sigma_3 \\
\sigma_4 \\
\sigma_5 \\
\sigma_6
\end{bmatrix} =
\begin{bmatrix}
C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{44}
\end{bmatrix}
\begin{bmatrix}
\epsilon_1 \\
\epsilon_2 \\
\epsilon_3 \\
\epsilon_4 \\
\epsilon_5 \\
\epsilon_6
\end{bmatrix}
\] (4.1)

Because of cubic symmetry, AlON has three independent elastic constants. We use \( C_{11} = 308.45 \) GPa, \( C_{12} = 119.61 \) GPa, and \( C_{44} = 163.94 \) GPa in simulations, and these constants are estimated by DFT calculations [96].

Anisotropic crystalline may have strong variations of elastic properties with the orientation of the direction in which they are loaded. For example, Young’s modulus of Silicon has
possible values between 130 to 188 GPa [97]. Variation of Young’s modulus and other elastic constant for different directions are characterized in theoretical work [98], in which directional dependence of the elastic modulus along a direction of interest can be described by the following equation:

\[
\frac{1}{E_{[hkl]}} = \frac{\alpha^4}{E_1} + \frac{\beta^4}{E_2} + \frac{\gamma^4}{E_3} - 2 \left( \frac{v_{23}}{E_2} \beta^2 \gamma^2 + \frac{v_{31}}{E_3} \gamma^2 \alpha^2 + \frac{v_{12}}{E_1} \alpha^2 \beta^2 \right) + \frac{\beta^2 \gamma^2}{G_{23}} + \frac{\gamma^2 \alpha^2}{G_{13}} + \frac{\alpha^2 \beta^2}{G_{12}}
\]  

(4.2)
in which \([hkl]\) is the direction of interest, three parameters \(\alpha\), \(\beta\), and \(\gamma\) are the directional cosines of the \([hkl]\) direction (the cosines of the angles between the direction \([hkl]\) and the x, y, z axes). The 1, 2, 3 subscripts in Eq. (4.2) are used to designate the directions of material coordinates. For example, \(E_1\) is the effective modulus along \([100]\) direction. This equation maps an unit sphere surface, which represents the material orientation, into an effective modulus surface. Notice that we use the Miller index notation [99]: \([ijk]\) indicates the direction of a vector, and \(<ijk>\) indicates the family of symmetric direction vectors.

Within a cubic crystal, \([100]\), \([010]\), \([001]\) directions are aligned with x, y and z axes (or 1, 2, 3) axes.

Eq. (4.2) can be simplified because AlON has cubic spinel structure [99]:

\[
\frac{1}{E_{[hkl]}} = \frac{1}{E_1} \left( \alpha^4 + \beta^4 + \gamma^4 \right) - \left( \frac{2v_{12}}{E_1} + \frac{1}{G_{12}} \right) \left( \beta^2 \gamma^2 + \gamma^2 \alpha^2 + \alpha^2 \beta^2 \right)
\]

(4.3)

The effective Young’s modulus (Fig.4.1) for AlON is obtained by subsisting material properties of AlON into Eq. (4.3). The \(<100>\) directions have the smallest modulus represented by blue, while \(<111>\) directions have the largest value, shown in red.
Figure 4.1: The tension coefficient surface (effective modulus along different orientations) for single-crystal AlON (left). The variation of the micromodulus function with orientation (right). Results produced by matching of strain energy densities for two different simple deformation modes.

4.2 Peridynamic model for single-crystal cubic elasticity

Until now, peridynamic models for elastic materials have used the strain energy density to calibrate the parameters in the PD model to the measurable material properties of the elastic bodies investigated. This is normally done by computing the strain energy density for a number of simple deformation modes, and equating those with the values produced by a classical elastic model. From such equations, one can determine the peridynamic bond stiffness in terms of elastic moduli.

We have tried this approach also for the crystals with cubic anisotropy by first assuming that the PD bond micromodulus surface has a similar shape as the tension surface of a cubic crystal:

\[
\frac{1}{c(\alpha, \beta, \gamma)} = \frac{A_1}{E}(\alpha^4 + \beta^4 + \gamma^4) + A_2 \left(-\frac{2v}{E} + \frac{1}{G}\right) \left(\beta^2\gamma^2 + \gamma^2\alpha^2 + \alpha^2\beta^2\right) ,
\]

(4.4)
In Eq. (4.4), the constant $A_1$ and $A_2$ have to be determined. A first attempt to determine these constants was to match the elastic strain energy density that results from a simple stretch along [100] direction, and a simple shear in a plane perpendicular to the [110] direction. This procedure produced values for the $A_1$ and $A_2$ which, when used into Eq. (4.4) results in the micromodulus surface function shown in Fig. 4.1. With this micromodulus, we then compute the actual longitudinal wave propagation speed along different directions in the single crystal peridynamic model. The results obtained for the wave propagation speeds along [100], [110] and [111] directions were undistinguishable from each other, whereas the theoretical values indicate waves propagate about 10% slower in the [100] direction than in the [110] direction, which is about 4% slower than the [111] direction (see Table 4.1).

<table>
<thead>
<tr>
<th>Direction</th>
<th>Wave speed (m/s)</th>
<th>Theoretical (m/s)</th>
<th>PD model (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>[100]</td>
<td>9227</td>
<td>10638</td>
<td></td>
</tr>
<tr>
<td>[110]</td>
<td>10236</td>
<td>10638</td>
<td></td>
</tr>
<tr>
<td>[111]</td>
<td>10654</td>
<td>10638</td>
<td></td>
</tr>
</tbody>
</table>

Because in dynamic fracture of brittle systems elastic wave propagation is the main cause of damage initiation and propagation (see e.g. [4]), it is critical that we are able to match, in the PD model, the known dependency with the orientation of the cubic crystal, of the wave propagation speeds. Therefore, we introduce a new strategy for computing coefficients $A_1$ and $A_2$ in 4.4 that gives the micromodulus function along an arbitrary direction of the unit sphere as follows: solve a least-squares minimization problems in which the variables are $A_1$ and $A_2$, and the objective function is the least-squares error between the theoretical and the PD model-computed longitudinal-wave propagation speed along the three directions shown in Table 4.2. In detail, this is performed as described below:

- Generate a starting guess for $A_1$ and $A_2$ (randomly selected inside a given range);
• Solve the PD model with these values to compute the wave propagation speed for a sudden loading of the single-crystal sample of (0.2 x 0.2 x 0.2 mm). In the PD simulation, a single crystal cubic structure (0.2 x 0.2 x 0.2 mm) is created to calculate wave speed. The cube center is the origin of the coordinate system to preserve computational symmetry. The cubic structure is uniformly discretized in material points with spacing 0.005 mm. Horizon size is 20 µm (about 1/10 of single-crystal sample size) to prevent erroneous homogenization caused by large horizon size with respect to the sample size. The Velocity-Verlet algorithm is implemented to integrate the PD equations in time. The maximum critical time step is 5 ns according to Courant-Friedrichs-Lewy (CFL) approach [100], and a 2 ns time step is used, for better accuracy, in the PD solutions performed during the optimization step (see below).

• After applying forces on the top surface of the cubic structure, stress waves are generated in the structure. To decrease the influence of peridynamic surface effects, the wave speed is estimated by monitoring two material points on the cross section shown in Fig. 4.2. Point 1 is at the center of the cubic and point 2 is 2δ away from the bottom surface. The wave speed is estimated by equation (4.5):

\[
V^{PD} = \frac{y_2 - y_1}{t_2 - t_1}
\]

in which, \(y_1\) and \(y_2\) coordinates of these two points along wave propagation direction, \(t_1\) and \(t_2\) are times of wave arrivals at these locations.

• Evaluate the objective function that minimizes the departure of these wave speeds from the corresponding theoretical ones:

\[
\min_{A_1, A_2} \sum_{i=0}^{3} (V_i^{PD} - V_i^T)^2
\]
where $V_i^{PD}$ and $V_i^{T}$ are longitudinal wave speed calculated by PD and the theoretical approximation [101] along the [100], [110], and [111] directions, respectively. Here,

$$V^T = \sqrt{\frac{E(1-v)}{\rho(1+v)(1-2v)}}$$

(4.7)

- Use a Simulated Annealing (SA) [102] optimization algorithm to generate the next pair of $A_1$ and $A_2$ values. The convergence history is shown in Fig. 4.2. We also used Gradient-based optimizers but those tended to get stuck in local minimizers. Genetic Algorithms have also been tried but they were significantly less efficient than SA results and also had problems with local minimizers.

With this procedure, we now obtain a micromodulus surface as in Fig. 4.3. With this micromodulus function, the PD model gives the wave speeds along the three directions [100], [110], and [111] shown in Table 4.2. The separation between the computed speeds is similar to the theoretical trend for these values: the slower [100] direction, the intermediate [110]
direction, and the fastest [111] direction.

Figure 4.3: Micromodulus surface for the PD single-crystal AlON model ($\delta = 20 \, \mu m$) constructed based on matching wave propagation speeds along three different directions [100], [110], [111].

Table 4.2: Longitudinal wave speed in single-crystal AlON along three directions

<table>
<thead>
<tr>
<th>Direction</th>
<th>Theoretical (m/s)</th>
<th>PD model (m/s)</th>
<th>relative error</th>
</tr>
</thead>
<tbody>
<tr>
<td>[100]</td>
<td>9227</td>
<td>9615</td>
<td>4.21%</td>
</tr>
<tr>
<td>[110]</td>
<td>10236</td>
<td>10135</td>
<td>0.99%</td>
</tr>
<tr>
<td>[111]</td>
<td>10654</td>
<td>10417</td>
<td>2.22%</td>
</tr>
</tbody>
</table>

4.3 Peridynamic model for a polycrystalline material with cubic symmetry

The flowchart in Fig. 4.4 shows an algorithm to determine the micromodulus of peridynamic bonds for polycrystalline materials. By using the coordinate system of the grain in which the node at one end of the bond resides, we compute the orientation of the peridynamic bond with respect to the grain in which this node resides: $\xi' = g\xi$ (see Fig. 4.4 and the transformation matrix $g$ below it).
Using the new bond vector $\xi'$, its micromodulus $C(\xi')$ can be computed based on the single-crystal PD model described in section 4.3. This micromodulus value will be used to calculate the peridynamic force in the bond unless the second node of this bond is in a different grain. When this happens (the other node is in a different grain), we calculate the micromodulus $C(\xi'')$ by using the bond’s orientation relative to the second grain $\xi'' = \tilde{g} \xi$ (in which the second node resides). Here, $\tilde{g}$ is the transformation matrix of the same bond but using the Euler angles of the second grain.

The smaller value of these two micromoduli is then assigned as the micromodulus of the bond crossing the grain boundary. The reason behind this selection is that grain boundaries are amorphous and thus likely to exhibit a softer elastic behavior than the individual grains. Note that this is only one possible option for the selection of micromoduli for bonds that cross grain boundaries, including those based on actually measuring the modulus of grain boundary, if available.

Remark: The bond-based model has limitations in representing all of the elastic properties of an anisotropic solid, and it would only approximate the elastic constants. A state-based PD model [32] can remove these limitations but it comes with a larger computational cost. In this chapter, our focus is on first understanding the mechanisms of brittle failure in the dynamic failure process of polycrystalline materials, and for that, having an exact match of the elastic constant is secondary.
4.4 Problem Setup and Convergence Results

4.4.1 Problem setup

For our quantitative comparison with experimental results on dynamic fracture in polycrystalline ceramics, we focus on the edge-on impact (EOI) experiments from [30]. The experimental sample size is 10 x 10 x 1 cm (see Fig. 4.5.a). The longitudinal wave reaches the side opposite to the impact surface of the sample in about 10 μs after the impact.

For simulations, we generate the Voronoi tessellation with random grain orientation using Neper [103]. Using the data generated by Neper (coordinates of Voronoi cells seeds), we create a uniform grid and associate each node with the grain to which it belongs. The average grain size is 200 μm in the simulation. Note that the grains in the AlON sample used in the experiments from [30] have sizes varying between 150 to 250 μm. With these realistic grains sizes in the model, the current serial version of our 3D code allows us to simulate a sample...
size much smaller (2.5 x 2.5 x 0.25 mm) than the one in the experiments. However, we will scale the applied loading so that the applied stress from the impact is similar to the ones reached in the experiments. Thus, we use a computational model with around 190 grains, shown in Fig. 4.6a.

We apply loading over a region to mimic a cylindrical impactor with radius 1.2 times of the sample thickness, similar to the one in EOI experiment (see Fig. 4.6b). Typical stress levels in the impact experiment are to be between 4 GPa and 30 GPa depending impact speeds, impactor and target materials. We select to apply 4 GPa of pressure (applied suddenly as body force density at nodes in the loading zone, and maintained constant in time for the duration of the simulation). This corresponds roughly to the pressure generated by the impact velocity of 400 m/s used in the experiments. The total simulation time is 0.3 µs, which is sufficient for damage to propagate over most of our computational sample size. A conservative time step was estimated to be 0.5 ns based on the equation:

$$\Delta t_{crit} = \frac{\Delta x}{c} \tag{4.9}$$

where $\Delta x$ is the node spacing and $c$ is the longitudinal wave speed. For the computations in this section we use the following material properties [104]: $C_{11} = 308.45$ GPa, $C_{12} = 119.61$ GPa, and $C_{44} = 163.94$ GPa.
4.4.2 Convergence study in terms of damage patterns

We perform a convergence study in terms of the damage patterns obtained by using smaller and smaller horizon sizes (and correspondingly finer and finer grids). This is $\delta$-convergence [50], in which the ratio $m = \delta / \Delta x$ is maintained constant as the horizon decreases. If the horizon size is in the range of the grain size, the effective behavior will be “averaged” with nearby grains, and there is little difference between the response of a polycrystal, single crystal, or isotropic material (see left column in Fig. 4.7). Apparently, the horizon size needs to be sufficiently small, compared with the average grain size, in order to capture the characteristics of failure in polycrystalline materials. We choose three cases:

- Case 1: horizon size is 2/5 of the average grain size: $\delta = 80 \, \mu m$ (grid spacing $\Delta x = 20 \, \mu m$);
- Case 2: horizon size is 1/5 of the average grain size: $\delta = 40 \, \mu m$ (grid spacing $\Delta x = 10 \, \mu m$);
- Case 3: horizon size is 1/10 of the average grain size: $\delta = 20 \, \mu m$ (grid spacing $\Delta x = 5 \, \mu m$). This case leads to about 12.5 million nodes in the discretization.
Using these parameters, we determine, for each horizon size and discretization, the corresponding micromoduli following the procedure discussed in section 4.3. With the obtained micromodulus functions, we first test the wave propagation speed in the sample to compare with the theoretical values. The results are shown in Table 4.3, indicating very good matches with the theoretical values, computed based on the elastic parameters from reference [96].

Table 4.3: Longitudinal wave speed in single-crystal AlON along three directions for different horizon sizes. Relative errors from classical theoretical are shown in parentheses.

<table>
<thead>
<tr>
<th>Direction</th>
<th>Theoretical (m/s)</th>
<th>Peridynamic (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$\delta = 80 , \mu m$</td>
</tr>
<tr>
<td>[100]</td>
<td>9227</td>
<td>9350 (1.33%)</td>
</tr>
<tr>
<td>[110]</td>
<td>10236</td>
<td>10141 (0.93%)</td>
</tr>
<tr>
<td>[111]</td>
<td>10654</td>
<td>10588 (0.62%)</td>
</tr>
</tbody>
</table>

Figure 4.7: Damage index at 0.3 $\mu s$ on the front surface of the sample. Horizon is 2/5, 1/5, and 1/10 of the average grain size (200 $\mu m$) for each column. From top to bottom, each row shows results with an isotropic, single grain, and polycrystalline model, respectively.
The surface damage produced for the three different horizon sizes and for three different material models (isotropic - using elastic properties of polycrystalline AlON, single crystal AlON with material coordinates same as the sample coordinates, and the polycrystalline AlON model with 190 grains) are shown in Fig. 4.7 at the end of the 0.3 µs total simulation time.

Damage in the coarsest model (δ = 80 µm) shows a large damage zone and some isolated cracks. By decreasing the horizon, the area of fragmentation damage shrinks while localized cracks take that space. Overall, the total failure (fragmentation and localized cracks) areas stays about the same for each material type under δ-convergence (follow rows of figures in Fig. 4.7).

The main damage characteristics, a highly fragmented zone, and localized cracks, are already present in the solution with the coarsest 80 µm horizon size, but with this coarse resolution differences between different material models (isotropic, single crystal, polycrystal) are small. As the horizon size is decreased to a fraction of the average grain size, we start to converge towards a clearly identifiable zone of massive failure, from which localized cracks sprout. Some localized cracks are also seen around the edges. Observe, again, that for each material type, the extent of the combined fragmentation zone and localized fractures is constant. We can consider that, in terms of damage patterns, the PD results converge. In the next sections, we will use the horizon δ = 20 µm and a corresponding grid spacing of ∆x = 5 µm to quantitatively compare the simulation results with those from experiments and also to explain the reasons behind the observed failure behavior.
4.5 Comparison Between Simulation Results and Experiments

4.5.1 Damage evolution: coherent failure front and localized cracks

The strain energy density and damage results are shown in Fig. 4.8 illustrate the evolution of the failure process from the EOI simulation (see movie 3 and 4 in supplementary materials). The strain energy imparted by the EOI travels through the structure and eventually damages the material which fails in mixed trans and intergranular fracture. The failure front leaves behind material that is shattered to small fragments (individual nodes are fully separated from all of their neighbors when damage reaches value 1 and the strain energy in these regions drops to zero since there are no bonds to be strained associated with these damaged nodes.

![Fig. 4.8: Strain energy density (top row) on the front surface, damage index (middle row) on the front surface, and damage index of a cut view (bottom row) at 0.05 μs, 0.10 μs, 0.15 μs, 0.20 μs, 0.25 μs, and 0.30 μs from the time of impact. Microstructure of the sample is overlapped on the damage maps. Computations performed with δ = 20 μm. All subsequent damage and strain energy plots use the same legends for the color scheme.](image-url)
Two stages of damage progression can be identified from these simulation results: in the first one related to a fast moving failure front that causes massive fragmentation, and the second one is the transition from the massive failure front to a slower front of localized cracks that sprout from the edges of the highly fragmented regions. The first stage is seen in first three columns in Fig. 4.8, while the second is observable from the last three columns shown in Fig. 4.8. These two stages are observed in experiments (see Fig. 4.5 and reference [30]).

It is interesting to also notice the evolution of damage shape on the side surface: at the early stages, damage grows, bounded by Hertz-cone like shape, with a flat front, tracking closely the strain-energy density map. By 0.1 µs, we already notice a transition in this shape, with the growth in the \( y \)-direction becoming slow, while the mid-line growth in the \( x \)-direction is much faster; this leads to an “artichoke”-like shape for the highly damaged region. At about this time, the propagation speed of the main damage front drops suddenly (see section 4.5.3), and localized cracks start to sprout from the main damage front. The propagation of the massively damaged region continues, but at a much reduced pace, while the localized cracks spread and run faster than the coherent damage front. By 0.2 µs, the coherent damage front has reached close to its final shape, while the localized cracks continue to propagate at almost constant speed (see section 4.5.3).

The final shape and structure of the computed surface damage are remarkably similar to that seen in the experiments (see Fig. 4.5.b): an “artichoke”-like shape of the highly damaged material, from which localized cracks spring out.

### 4.5.2 Damage on surface and in the bulk

The experiments show a significant difference between the shadow graph results (that “overlaps” damage through the sample thickness) and the reflected light results (see Fig. 13 in [30]). This indicates that there is some difference between damage on the surface of the sample and damage through the thickness of the sample. We now verify whether this is captured
by our peridynamic model.

We note that, given the sample size used in the computations, we have about 1-2 grains through the thickness of the sample. Nevertheless, the results in the top row of Fig. 4.9 do clearly indicate a significant difference between what happens on the sample surface and inside the sample. The time evolution of damage is similar between these two sections, however, damage seems to first happen on the surfaces and arrive at the center slice after some delay (see more on this in section 4.6). The damage in the center slice has less fragmentation than the outside surfaces, and these differences are expected to be even more pronounced in thicker samples with more grains through the thickness. The evolution of the strain energy density seen in the bottom row of Fig. 4.9 confirms the conclusion on the differences between the surface and center damage evolution, that the center of the sample is more “protected” from damage than its surfaces.

Figure 4.9: Damage index (top row) and strain energy density (bottom row) for material points in the middle $xy$-plane section (left) and the front surface (right) at 0.30 $\mu$s.
4.5.3 Supershear damage propagation and subsonic localized cracks

Another quantitative comparison with experiments is on estimating the propagation speed of the primary damage front (highly damaged region) and that of the secondary fracture front (localized cracks that emanate from the primary damage front once the energy intensity in the sample reduces).

The forward difference approximation between two consecutive data outputs of damage information is used to estimate the propagation speed of the primary damage front and the secondary fracture front. For example, to calculate the propagation speed of the primary damage front, we select a damage index of 0.5 and monitor (manually) its advancement along the $x$- and $y$-directions in time. The horizontal and vertical propagation speeds are calculated using the coordinates of nodes with the selected damage index value sitting at the front. Similarly, we estimate the propagation speeds of the secondary fracture front by observing the growth of two localized cracks using same critical damage index.

Fig. 4.10 shows the propagation speed for the primary damage front along $+x$ and $-y$ directions, and the crack propagation speed for two of the localized cracks. We obtain an average value of about 8.7 km/s for the highly damaged front along $+x$ direction and 2.6 km/s along $-y$ direction. The damage velocity measured in experiments is 8.4 km/s [30].

Interestingly, we obtained a drastically lower speed of propagation of the individual cracks emanating from the main failure front: about 4.8 km/s for the one propagates along $+x$ direction, and 4.6 km/s for the one growing vertically. The experimental results give the crack velocity a value of 4.4 km/s [30]. Notice that in experiments [30], the longitudinal wave speed for AlON is 10.2 km/s, which is close to our estimation. Shear wave speed in polycrystalline AlON is about 5.8 km/s. Note that the Rayleigh wave speed $c_R$ corresponding to an isotropic material that has the same elastic constants as polycrystalline AlON would be about 4.9 km/s based the following equations ([105]):
Figure 4.10: Propagation speed of damage front and localized cracks in (a). In (b), damage map at 0.3 μs and arrows indicating the directions used for measuring the damage front propagation speed and the localized cracks selected for measuring their speed.

$$c_R \equiv (2 - M_2^2)^2 - 4 \sqrt{(1 - M_1^2)(1 - M_2^2)} = 0$$

in which,

$$M_1 = \frac{c_R}{c_1}, M_2 = \frac{c_R}{c_2}$$

where $c_1 = \sqrt{(\lambda + 2\mu)/\rho}$, $c_2 = \sqrt{\mu/\rho}$, and $\lambda$, $\mu$ are the Lame’s constants. The Rayleigh wave speed is the real root of this equation in the range $0 < c_R < c_2$.

Therefore, we can say that the primary failure front is supersonic (supershear), while the individual cracks are subsonic, but are still growing at a rather high fraction of the (equivalent) Rayleigh wave speed (see [60]).
4.6 Understanding the evolution of damage

In this section we explain the reasons behind the supershear propagation speed of the primary failure front, and the dramatic change in propagation speed from that of the primary failure front to that of the localized cracks sprouting from it.

Waves interaction and reinforcement are the primary reasons for dynamic fracture and damage in brittle materials. We will show that the coherent damage front, which leads to regions of as highly fragmented material and is traveling at supershear speed (∼ 8.4 km/s), is caused by a wave front like the second wave front seen in a snap-shot from [30] and visible in Fig. 4.5 above. As stated in [30]: “The formation of the second wave front is caused by the geometry of the specimens and is due to the initiation and superposition of waves, generated at the side surfaces of the specimens”. The interaction of this wave front with the free surfaces of the sample, that bound the thickness direction (the $xy$ surfaces perpendicular to the $z$-direction, see Fig. 4.6) leads to damage. These surfaces are the ones shown in Figs. 4.7, 4.8, 4.10.

To understand the evolution of damage, we monitor the in-plane nodal velocities and damage index for nodes in the center $xz$-plane cross-section (see Fig. 4.11). This cross-section has the loading on its left boundary.

4.6.1 Evolution of damage in the isotropic material

Because the evolution of damage from EOI for the polycrystalline material is similar, to a certain degree, with that of the isotropic case (see Fig. 4.7), we investigate the isotropic sample, modeled using the elastic properties of polycrystalline AION. This study will also allow us to identify which parts of the damage evolution are influenced by the specific microstructure and which parts are independent of it.

Since the progression of damage in the material can disrupt/disturb wave propagation,
we also perform simulations in which damage is not permitted. In Fig. 4.11, the rows of plots show the $xz$-component of the nodal velocity vectors. The color mapping for the first two rows is the $v_z$-magnitude, while for the third row is the damage index value. The top row of plots is for the case in which damage is suppressed. The third row of plots gives the damage index for the results corresponding to the second row.

The results in Fig. 4.11 support the following description for the initial stages of damage evolution in the sample’s center through-thickness cross-section:

- Damage initiates at the corners of the cross-section (corresponding to the front and back surfaces of the sample) because motion for nodes in these regions leads to relative elongations larger than the critical ones;

- The regions with high $z$-direction nodal velocities in this cross-section correlate well
with the regions where damage develops (see Fig. 4.11);

- The leading edges of wave fronts with high $z$-direction velocities (regions with high local shear), generated from the corners of the cross-section, form an angle $\theta$ with the sample surfaces (see the angle marked by a black dash-dot line Fig. 4.11) that stays constant in time, independent on whether damage is allowed to form or not;

- A wave front, similar to the “second wave front” mentioned in [30], determines the propagation speed of the primary damage front, $v_{df}$, on the sample surfaces. The through-thickness propagation of this wave front forms the constant-in-time angle $\theta$ and causes the growth of triangular-shaped damaged regions that advance with a normal velocity $v_{dfn} = v_{df} \times \sin \theta$ (see Fig. 4.11). The through-thickness damage zones eventually meet with one another, at a time that is dependent on the sample thickness.

In order to test whether the above observations are independent of the geometry, we create another sample with twice the thickness of the original one, so that the new sample thickness is 0.5 mm. The same material properties, horizon size ($\delta = 20\mu m$), and discretization as in the previous test were used. The wave propagation in the center cross-section in the $xz$-plane is illustrated in the plots in Fig. 4.12 for samples in which damage is precluded or is allowed. By comparing the results in Figs. 4.11 and 4.12, we observe that the early stages of damage evolution are independent of the thickness of the sample: the same waves and damage patterns are observed and the angles between the front of the high magnitude nodal $z$-direction velocity regions, that grows through the thickness, and the sample surfaces, are identical between the two different samples.

As time progresses, complex waves interactions with the sample boundaries lead to damage that is dependent on the sample thickness, for example. Wave interactions are also responsible for the observed change in shape of damage noticed on the side surfaces of the sample (see section 4.5.1 and the “artichoke”-like shape of damage).
Figure 4.12: Thicker sample: velocity vectors in the $xz$-cross-section for an isotropic material with (bottom two rows) or without (top row) damage showing time evolution of wave propagation and damage. The red circle in the lower left corner shows the horizon size ($\delta = 20\mu m$) relative to the sample size.

We calculate velocities of the primary damage and isolated cracks of the isotropic model (see section 4.4.2 and top-right plot in Fig. 4.7). The propagation speed for the primary damage front and the front of isolated cracks for the horizontal direction, in this case, are shown in Fig. 4.13). The average propagation speed for the primary damage and localized cracks are 8.7 km/s and 3.9 km/s, respectively. Notice that we used the damage index value of 0.5 to monitor these fronts and calculate their propagation speed (see Figs 4.10 and 4.13).

Behind the primary damage front, we also observe the motion of another damage front that leads to full fragmentation (damage index = 1.0) on the side surfaces of the sample, in both the polycrystalline and isotropic models (see 2nd and 3rd rows of plots in Fig. 4.8, and 3rd row in Fig. 4.12). In Fig. 4.13 we show the propagation velocity of this full fragmentation front in the isotropic material case (computed as for the other fronts but monitoring nodes with damage index of 1). Its average velocity is 6.1 km/s. This is very close to the shear wave speed of 5.8 km/s in an isotropic material with equivalent elastic properties as the polycrystalline AlON. The shear wave speed carries much higher energy compared with the
longitudinal wave. The authors of [30] proposed a similar hypothesis to explain the behavior observed in their experiments (see Fig. 2 in [30]). We conclude that the shear wave is the reason of full fragmentation.

4.6.2 Evolution of damage in the polycrystalline material

In this section, we focus on the differences seen in terms of damage pattern between the isotropic material and the polycrystalline material under EOI. The polycrystalline sample is the AlON material discussed above (see Fig. 4.6), and the isotropic one uses the effective material properties of polycrystalline AlON (see section 4.4.2 and Fig. 4.7).

First, we discuss damage in the through-thickness section used in the previous section for the isotropic and polycrystalline models. Fig. 4.14 shows the damage index maps at 0.15 µs. The damage profiles are similar, especially over the left half of the cross-sections. Some small differences are observed, likely caused by the microstructure of the polycrystalline sample. These differences would be caused by the changes in the wave propagation introduced in
Figure 4.14: Damage index at 0.15 µs from time of impact over the xz-cross-section. (a): isotropic model; (b): polycrystalline model; (c): corresponding microstructure for the case in (b); (d): nodal velocities at 5 ns over the region shown in the square drawn in (c).

the sample by grain anisotropies and by the presence of grain boundaries. These material interfaces produce extra reflections and mode conversion of waves. The results (see Fig. 4.14) indicate that wave dispersion caused by the microstructure may protect against brittle failure (see also [106]). Notice the less damaged areas in the right half of Fig. 4.14b compared to Fig. 4.14a. At 5 ns, stress waves pass the first grain boundary, highlighted in Fig. 4.14c. The nodal velocities are shown in Fig. 4.14d over this region, demonstrate the existence of shear motion (for the y and z directions) across the grain boundary. Such deformation would not happen in the isotropic case, and this could explain, in part, how this “energy dispersion” mechanism may be protective for the polycrystalline structure compared with an, equivalent, isotropic sample.
Consider now the damage on the surface of the sample of the isotropic and polycrystalline samples. The final damage (at 0.3 μs) on the surface of both samples has a similar shape: “lotus flower” for the isotropic case, and “artichoke-like” for the polycrystalline sample (see Fig. 4.15). These shapes are bounded by a Hertz-cone (see Fig. 4.15). In both instances, the highly fragmented region is slightly longer along the loading direction (+x). As observed before along the middle cross-sections of the samples, the fully fragmented side surfaces are smaller in the polycrystalline case than in the isotropic case, supporting the previously mentioned idea that the presence of a microstructure is protective against dynamic failure.

Sprouting from the primary damage front (which is caught up by the highly fragmented region at the time shown in Fig. 4.15), isolated/localized cracks propagate in both samples, but in different ways. In the polycrystalline case, many of the isolated cracks grow along grain boundaries, with some growing transgranular. In the isotropic case, the isolated cracks are smooth and curve back towards the center of the sample, likely because reflection waves change their paths.

Propagation of the full fragmentation front in the polycrystalline model is complex. It is driven by the shear wave and influenced by grain orientation and grain boundaries. Observing snapshots in Fig. 4.8 and movies (movie 3 in supplementary materials), we find that full fragmentation first develops along grain boundaries in the primary damage region. Then, the fragmentation front grows into the grains, with varying speeds between the grains.

Note also that some cracks initiate from the boundaries of the sample (see snapshots in Fig. 4.8) and grow toward the inner regions. This type of cracks are also seen in the experiment (see Fig. 4.5). Edge cracks formed by waves in brittle materials, like glass, are discussed in detail in [107] for the case of direct impact on a glass plate.
4.7 Conclusions

The peridynamic model presented here provides quantitative predictions of the experimentally observed failure modes and propagation of damage characteristics in the Edge-On Impact (EOI) in polycrystalline AlON. The computational model matches the experimental results for the supershear propagation speed for the primary failure front and the subsonic propagation speed of the localized cracks that grow once the main failure front loses strength. The shape and structure of damage are very similar to those seen in the experiments. By analyzing the peridynamic results, we are able to explain the reasons behind the particular type of damage evolution in the EOI. Damage is found to initiate from the edges of the sample and is driven by a wave front that propagates on the sides of the sample but also through the thickness, at an angle. Full fragmentation of the already damaged material happens on the side surfaces of the sample, and partially through the sample thickness, because of shear waves.

We also contrast damage in the polycrystalline sample with damage in an equivalent isotropic material. We find that the presence of microstructure can be “protective” against dynamic fracture and damage because the dispersion of waves limits the progression of the failure fronts.

The results point out that other dissipation mechanisms likely present in the EOI tests
in polycrystalline AlON (like twinning, plasticity, etc) may be second order effects in the evolution of damage and failure. The main ingredients used in the model developed here are: polycrystalline microstructure (represented using same average grain size like in experiments, but on a scaled-down sample size), 3D anisotropic elasticity, and brittle damage model. The advantage of the Peridynamic formulation for this problem rests in its ability of handling the evolution of damage in a natural way: extensive diffuse damage autonomously transitions to localized cracks when the conditions require it; trans and intergranular failure modes are captured without additional/special criteria.
Chapter 5  Prediction of crack nucleation sites of a cubic crystal superalloy

Fatigue cracking is the most common cause of structural failure in aircraft. Damage tolerant design or safety by inspection is a commonly used design method in industry, which predicts the crack propagation based on fracture mechanics and also needs periodic inspection. Comparing with crack growth simulation technique, which is mature and used in engineering practices, understanding the crack nucleation process and incorporating microstructure in design/lifing are still in the elementary stage [34]. Fatigue crack is caused by the crystal plastic strain localization. In high-cycle fatigue, applied stress is far below the yield stress. The well-known persistent slip bands (PSBs), which are carriers of plastic deformation, appear as cycle number increases. It is the microstructure inhomogeneities produces strain localization [35]. Investigating microstructure based lifing would: 1) benefits the design of crack nucleation resistant microstructure, 2) improves simulation of fatigue failure considering that the nucleation process usually takes 80% of the total life of high cycle fatigue [108], 3) guides material processing processes.

To describe the first stage of the fatigue failure, crack nucleation and crack initiation have been used interchangeably in engineering and scientific communities. We use crack nucleation in this chapter to describe the formation of grain level crack. It is well established that cracks nucleate at the material surface because these grain are less constraint compared with subsurface grains without considering the existence of precipitates, impurities, and inclusions [109]. In terms of grain size, many experimental works show that crack nucleate from large grains [110, 111, 112], the reason is that larger grain enables more slipbands formation. Grains with similar crystallographic orientation form “supergrains”, which allows
slip transmission across low angle grain boundaries [112]. This phenomenon was found in both Ni-based superalloy and Ti-alloys. Miao and co-authors [35] found that in a Ni-based superalloy, most crack nucleated from grain clusters which have misorientation less than 20°. Crack nucleation near the twin grain boundaries has attracted much attention. Earlier experimental works on twin boundaries cracks are performed on copper [113] and steels [114]. Recently, experiments [35] on the superalloy René 88DT at room temperature show that most crack nucleated near the Σ3 twin boundaries in surface grains with size three times larger than average grain size. Experiments at elevated temperature and analytical studies [115] show that elastic incompatibility plays a key role in stress localization in twin boundaries. Highest stress concentration is found parallel and slightly offset from the twin boundaries, and the concentration magnitude is about 8 times the macroscopically imposed strain [116].

Besides the development of experimental techniques, advanced computer science makes it possible to study microstructure based lifing. For example, we can largely improve computational efficiency by using advanced hardware, like GPGPU and Intel Xeon Phi Coprocessors for parallel programming. A recently published work [117] studies the influence of microscale material variability on macroscale by directly simulating 420 thousand grains within an I-beam using a massively parallel finite element code.

Three conventional techniques of simulating crack nucleation are molecular dynamics, discrete dislocation plasticity, and crystal plasticity. The molecular dynamics requires a relative small integration step size compare to the period of bond vibration. Another limitation is that computationally we cannot afford a sufficient number of atoms to simulate most engineering problems. The advantage of the discrete dislocation plasticity method is that it can capture the formation of persist slip bands, while the disadvantage is 3D anisotropic model is unavailable for materials like many superalloys [34]. Crystal plasticity is capable of capturing the heterogeneous plastic deformation, texture evolution, and dislocation
of metallic material under large deformation. Coupling crystal plasticity with finite element method is the most popular approach for understanding microscopic plastic deformation and crack nucleation. For example, Dunne et al [118] inserted a crystal plasticity region with the same microstructure from measurement into a homogenized finite element model and captured the locations of persistent shear bands and crack positions. However, the most likely predicted crack nucleation sites is not observed in the experiments. Clayton [119] combined the cohesive zone model with finite element crystal plasticity to simulate the crack nucleation and propagation in a 2D plane strain microstructure model. Special treatments are needed for classical mechanics based methods when cracks exist because deformation gradient and spatial derivatives, and the cohesive zone model only allow crack propagate along the element boundaries.

Peridynamics, a new non-local method, has been proposed to deal with dynamic fracture problems by Silling [1]. Peridynamics is a reformulation of the classical continuum mechanics equations that allows for a natural treatment of discontinuities in the solution by employing the concept of nonlocal interactions. Integration, rather than differentiation, is used to compute the total force density acting on a certain material volume, and deformation gradients are not used in the formulation [120]. A distinguishing feature of the peridynamic approach is that it allows for spontaneous formation, interaction, and growth of discontinuities in a consistent framework [3].

With this motivation, this chapter attempts to study the crack nucleation using peridynamics. Peridynamic simulation of polycrystalline materials is first mentioned in [33], in which the crack pattern influenced by a critical stretch of bonds on grain boundaries are discussed. Ghajaria et al. [121] proposed a transversely isotropic model under plane stress and plane-strain conditions and used to simulate dynamic brittle fracture of 2D polycrystalline microstructures. Sun and Sundararaghavan [122] proposed a 2D cubic plasticity based on the state-based peridynamic framework. In this chapter, a 3D cubic elastic model is used to predict the
In the present work, a 3D bond-based peridynamic model for polycrystalline materials with cubic symmetry grains [123] is used to simulate crack nucleation sites in a material system with a synthetic microstructure (the René 88DT model). The material system studied in this work is the René 88DT microstructure of polycrystalline Ni-based superalloy, widely used for aeroengine turbines. We simulate strain concentration sites from twin grain boundaries in the synthetic model and compare results with commercial finite element (FE) software for validation. Strain concentration sites captured by the peridynamic polycrystalline model are similar to those produced by a FE simulation. Most concentrations are along the twin grain boundaries. The peridynamic model allows nucleation of damage sites from the complicated strain fields as well as their further propagation and coalescence through full development of micro-cracks and cracks. We demonstrate nucleation of damage in this material using a peridynamic fatigue failure model.

### 5.1 Simulation results and validations

The peridynamic cubic elasticity model proposed in Section 4.3 is used to simulate crack nucleation in René 88DT, which has cubic symmetry. Three elastic constants are needed to describe the cubic elasticity: $E_x = E_y = E_z = 97.62$ GPa, $\nu_{xy} = \nu_{yz} = \nu_{zx} = 0.41$, and $G_{xy} = G_{yz} = G_{zx} = 108.00$ GPa, here we assume that a grain with axes at [100], [010], and [001]. In this section, we validate the model by checking the effective modulus along different directions, strain across the grain boundary, and strain concentration sites in a polycrystalline model. Finally, crack nucleation is simulated by using the fatigue cracking model.
5.1.1 Modulus variation in one grain with different orientations

As pointed out in [123], elasticity is a fundamental component in simulations of noncrystalline materials, so two parameters $A_1$ and $A_2$ in Eq. (4.4) are obtained by matching moduli between PD and theoretical values along three group of directions ([100], [110] and [111]) in a single crystal sample. Table 5.1 compares effective moduli of the ([100], [110], and [111]) directions in a single grain between the analytical values from classical cubic elasticity and values by numerical solutions of the peridynamic models using three different horizon sizes (and the corresponding grids for horizon factor $m = \delta / \Delta x = 4$. The uniform discretizations with a horizon factor $m = 4$, produced results that matched experimental observations in Edge-on impact test, when the horizon size was sufficiently small relative to the grain size (see [123]). Differences of effective moduli between peridynamic simulation and analytical values decrease as the horizon size $\delta$ decreases from 3 $\mu$m to 1.6 $\mu$m. These results show the $\delta$–convergence, as defined in [50].

Table 5.1: Effective moduli of single grain calculated by the peridynamic cubic elasticity model. Relative errors from classical theoretical are shown in parentheses.

<table>
<thead>
<tr>
<th>Directions</th>
<th>Euler angles</th>
<th>Analytical</th>
<th>Effective modulus (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>PD $\delta=3.0$</td>
<td>PD $\delta=2.0$</td>
</tr>
<tr>
<td>100</td>
<td>(0, 0, 0)</td>
<td>97.6</td>
<td>102.2 (4.71%)</td>
</tr>
<tr>
<td>110</td>
<td>(0, 45, 0)</td>
<td>188.3</td>
<td>186.4 (1.01%)</td>
</tr>
<tr>
<td>111</td>
<td>(0, 55, 45)</td>
<td>271.8</td>
<td>277.8 (2.21%)</td>
</tr>
</tbody>
</table>

Note: Euler angle in degrees based on ZXZ convention

5.1.2 Strain variation across a grain boundary

Microstructure, including grain orientation and grain boundaries, is another key component in simulations of noncrystalline materials. The algorithm for assigning grain orientation in the peridynamic simulation is discussed in [123]. This section focuses on how to describe grain boundaries, which are interfaces in noncrystalline materials, in the peridynamic simulation.
Similar to other non-local methods, simulating the interface is an issue to peridynamics because a peridynamic bond may links two material points with different material properties, as a bond $\xi(x, q)$ connects material point $x$ and $q$ in Fig. 5.1. To calculate the micromodulus of a bond crosses interface, averaged material properties and bond micromodulus are used in following simulations. As shown in Fig. 5.1, two materials within the horizon of material point $x$. The effective material properties is calculated based on

$$E(x) = \frac{E_1 V_1 + E_2 V_2}{V_1 + V_2},$$  \hspace{1cm} (5.1)

where $E_1$, and $E_2$ are Young’s moduli of two materials and $V_1$, $V_2$ are volume (or area for 2D case) of these two materials within horizon of $x$. Like Young’s modulus, other material properties are also calculated similarly. The micromodulus of the bond $\xi(x, q)$ is calculated using volume weighted moduli

$$c'(x, q) = \frac{c(x) + c(q)}{2},$$  \hspace{1cm} (5.2)

in which, $c(x)$, and $c(q)$ are calculated by Eq. (2.7).

A 3D sample with two cubic grains along the z-axis is simulated to validate the peridynamic simulation with grain boundaries. Geometry of each grain is 10x10x10 $\mu$m. The discretization for this peridynamic model has a uniform grid with spacing between material points of 0.5 $\mu$m, and a horizon size is 2 $\mu$m. The sample is in tension by fixing nodes on the right
surface and applying 1 MPa pressure on nodes on the left surface. Orientation of these two grains are (0, 0, 0) and (0, 45, 0), which produce effective moduli 97.6 GPa and 188.3 GPa respectively along the loading direction.

Strain along the center line of the sample is plotted in Fig. 5.2. As expected, the grain with smaller effective modulus has larger strain. Near the grain boundary, we can see the abrupt strain variation. Different from the sharp (discontinuous) drop of strain by ANSYS, peridynamic simulations give a smooth transition for strain between grains. As the horizon size decreases, we find a better match between the peridynamic simulations and ANSYS results in terms of strain in the grains. Also, the strain variation across the interface gets sharper with the smaller horizon size. The thickness of the variation region is about $2\delta$, which is similar to the influence region of a free surface.

We conclude that in order to obtain strains that have high gradients at a grain boundary, in a PD model we need to use a horizon size sufficiently small compared to the grain size. We note that the ANSYS solution is not necessarily the “true” solution, for the following reason: grain boundaries are never perfect straight mathematical lines (because of impurities, vacancies, misorientation, etc.), therefore one should not expect a mathematical discontinuity in the strain across a grain boundary.

Figure 5.2: Normal strain values along the center line across a grain boundary from ANSYS and the PD simulations
5.1.3 Strain concentrations sites of René 88DT

Figure 5.3: Microstructure of the synthetic model, which has 179 grains

We consider the following setup for analyzing the strain concentration sites in polycrystalline materials: a synthetic René 88DT model with 100 x 100 x 50 µm as shown in Fig. 5.3. This model has 179 grains with random orientation and most of them are twin grains. René 88DT has FCC microstructure, twins in this type of materials share Σ3 boundary, which is 60° rotation about the [111] direction. This microstructure is generated by DREAM3D [124] based on statistical data from experimental measurements. Voxel data from DREAM3D is then used to build a peridynamic model, so the peridynamic model has an uniform mesh (Δx = Δy = Δz). Three peridynamic simulations are performed using different horizon size, see parameters listed in Table 5.2. Nodes position in discretized models starts from the coordinate origin to 100, 100, 50 µm in 3D. The sample is in tension by applying force density, which is equivalent to 500 MPa pressure, on the top nodes (y = 100 µm) and fixing translational degree of freedoms of bottom nodes (y = 0 µm). To validate the peridynamic simulation results, an FE simulation is performed using ANSYS, and we will compare the strain concentration sites calculated by two methods. The FE model has about 2.69 million elements, 3.66 million nodes, and has same boundary conditions. Notice that because the
peridynamic model is nonlocal and no surface exists, so all boundary conditions are applied material points.

Table 5.2: Peridynamic parameters, node number and computational time of three discretization

<table>
<thead>
<tr>
<th>Horizon (µm)</th>
<th>Node spacing (µm)</th>
<th># nodes</th>
<th>Time used (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.0</td>
<td>0.75</td>
<td>1,167,474</td>
<td>5.8</td>
</tr>
<tr>
<td>2.0</td>
<td>0.50</td>
<td>4,000,000</td>
<td>11.7</td>
</tr>
<tr>
<td>1.6</td>
<td>0.40</td>
<td>7,812,500</td>
<td>24.6</td>
</tr>
</tbody>
</table>

As a nonlocal method, peridynamic simulations are computationally expensive compared with FE simulations. To save computational time, peridynamic simulations are accelerated by OpenACC for multicore CPUs. All simulation times listed in 5.2 are performed using 32 cores on a Linux machine with AMD Opteron 6272 CPU. Detailed parallel strategy is discussed in Section 3.2.4.

As discussed previously, cracks first nucleate on the free surface of samples under cyclic loading based on experimental observation, here we show simulation results of four free surfaces of the sample in Figs 5.4 and 5.5. Here we show a contour plot of $\varepsilon_y$, the normal strain along loading direction. All results are plot in same contour range: from 0.3% to 0.5%. In FE results of these figures, black lines represent grain boundaries. By comparing FE and peridynamic simulation results, we can find:

- strain concentration sites by two methods are almost identical except the bottom region where boundary condition applied on;
- peridynamic results have lower magnitude of strain values than FE;
- as expected, in both FE and peridynamic simulation results, most strain concentration are present at the twin grain boundaries;
Figure 5.4: Compare normal strain $\varepsilon_y$ on the front (first column) and back (second column) surfaces of the sample between FE (first row) and PD (second row) simulations.

Figure 5.5: Compare normal strain $\varepsilon_y$ on the left (first column) and right (second column) surfaces of the sample between FE (first row) and PD (second row) simulations.
To validate the PD model, here we also compare results in bulk between peridynamic and FE simulations, which show similar strain concentration as on the free surfaces. We select mid-plane along three axis of the sample and compare $\varepsilon_y$ of these planes, as shown in Figs. 5.6, 5.7 and 5.8. Microstructure information are provided in Figs. 5.6c, 5.7c, and 5.14e to show the strain concentration related to grain boundaries. Clearly, strain concentration sites in the peridynamic simulation are almost the same with FE results. It is worth noting that strain concentration sites near triple junctions are captured by peridynamic simulation, for example, the one near the top-right corner in Fig. 5.7b and another in the center of Fig. 5.14c. Different from results on the surfaces of the sample, no strain concentration can be found along twin boundaries in bulk. We can classify concentration sites into two categories:

1. concentration originate from edge of the mid-plane, which is consistent with observation that cracks nucleate from the surface, and these concentration sites are at the twin grain boundaries. For example, concentration sites at top and bottom edges in Figs. 5.6a, 5.6b, 5.7a, and 5.7b.

2. whole grains in strain concentration, as grains shown in Figs. 5.7a, 5.7b, 5.14a, and 5.14c. These grains are also twin grains.

Figure 5.6: $\varepsilon_y$ of the middle plane ($x = 50 \mu$m) in FE and PD, with microstructure.

The objective of this chapter is to show the effectiveness of peridynamic model on the prediction of crack nucleation sites. Fatigue crack of ductile materials starts from cyclic strain localization, and persistent slip bands appear at these localization sites. Classical
mechanics assumes that materials only have elastic deformation under hydrostatic pressure, in another word, plastic deformation is a result of deviatoric deformation, which is directly related to the von Mises stress/strain. In the simulation, the sample is in tension along the y-axis, so strain concentration sites shown by $\varepsilon_y$ indicates possible crack nucleation sites. We can show this by comparing results expressed in normal strain $\varepsilon_y$ and von Mises strain $\varepsilon_{vm}$, see Fig. 5.9. As expected, the contour plot between $\varepsilon_y$ and $\varepsilon_{vm}$ are about the same because the sample is loaded along the y-axis.

To quantitatively compare strain concentration in peridynamic results with FE results, we compare $\varepsilon_y$ along the three lines on a center plane ($y = 50 \, \mu m$) of the sample. These three lines are along the x-axis. The first line is on the front surface ($z = 50 \, \mu m$) of the sample, the second line is in the center ($y = 50 \, \mu m$ and $z = 25 \, \mu m$) of sample, and the third line is on the back surface ($z = 25 \, \mu m$) of the sample. For the peridynamic result, results are of peridynamic points on these lines. The FE results are obtained by selecting elements
within 5 µm distance around a line and mapping (ANSYS APDL *MOPER) results to it, because insufficient nodes exist along lines in FE model as a result of using graded mesh. Curves in these figures show the variation of strain across grains in the sample. Results of the largest horizon size (3 µm) show strong variation and large difference from ANSYS results, we can see slightly shifted strain concentration location and strain variation trend in some grains are different from peridynamic results by finer mesh. We get these discrepancies because inaccuracy description of the grain boundary caused by the coarse mesh. Using smaller horizon size 2 and 1.6 µm, peridynamic results are much closer to ANSYS results. Results by these two smaller horizons are almost same for most of these curves, while results by 1.6 µm horizon show a smaller difference between ANSYS results on the right-hand side of all three curves. By comparing peridynamic results of δ = 1.6 µm and ANSYS results along three lines, similarities are that:

- Strain variation in the center of the sample (see Fig. 5.12) are more than two times smaller than strain on the free surfaces (see Fig. 5.10, 5.11)

- Highest strain concentration is found in Fig. 5.11,
• strain concentration in peridynamic results have lower magnitude, which might be caused by using averaged micromoduli near grain boundaries. The largest difference exists in the first concentration point in Fig. 5.12, which is about 25%;

• larger differences between two methods are found near ends of these three lines, the largest error appears at $x = 100 \, \mu m$ in Fig. 5.11;

Figure 5.10: $\varepsilon_y$ along the interaction of $y = 50 \, \mu m$ and $z = 50 \, \mu m$. Vertical dashed lines and dash-dot lines indicate the position of the twin boundaries and grain boundaries along this interaction line. The PD horizon size is in $\mu m$.

Figure 5.11: Compare $\varepsilon_y$ between ANSYS and three PD simulation with different horizon size, along the interaction of $y = 50 \, \mu m$ and $z = 0 \, \mu m$. Vertical dashed lines and dash-dot lines indicate the position of the twin boundaries and grain boundaries along this interaction line. The PD horizon size is in $\mu m$. 
Figure 5.12: $\varepsilon_y$ along the interaction of $y = 50 \, \mu m$ and $z = 25 \, \mu m$. Vertical dashed lines and dash-dot lines indicate the position of the twin boundaries and grain boundaries along this interaction line. The PD horizon size is in $\mu m$.

5.1.4 Crack nucleation

Based on the static solution, we can predict the crack nucleation sites under using the fatigue crack model [29]. Implementation details of the fatigue failure model are discussed in chapter 3. In this section, we only use the first phase, which is the crack nucleation of the fatigue crack model. Parameters in the crack nucleation phase are calibrated by using the S-N curve data from an experimental work [125]. Fig. 5.13 shows data points from experiments in log-log plot and a linear fitted line for calibration.

The model with $2\mu m$ horizon size is adopted in the fatigue crack simulation. To save computational time, half of the original sample is used ($100 \times 100 \times 25 \, \mu m$) and the half model has the same back surface ($Z = 0 \, \mu m$). Loading conditions are same to the previous section but the magnitude of pressure is changed to 1000 MPa in the fatigue failure simulation. Also, a $0.5\delta$ thickness no-fail zone is assigned on the bottom of the sample. Results show that all damage is on free surfaces of the sample. Fig. 5.14 show damage maps and corresponding microstructure of the back surface ($Z = 0 \, \mu m$). Boundaries of the sample are illustrated by dashed lines in damage maps. Damage results are consistent with strain results in Fig. 5.5 because the model is linear elastic. Notice that most damaged nodes have damage index
smaller than 0.05 in all damage maps. On the left boundary of the damage maps, which is an edge of the sample, we can find two locations have largest damage index. The one near the bottom of the sample might be caused by the boundary condition. Another one would be a crack nucleation site. We can predict that a crack will be developed at this point and propagates along the twin grain boundary. Also, grain boundaries with high strain concentration have many damages material points. These grain boundary would be sources of cracks as observed in experiments.

The model with 2 \( \mu \)m horizon size is adopted in the fatigue crack simulation. To save time, half of the original sample is used (100 x 100 x 25 \( \mu \)m) and the half model has same back surface as the original full model (\( Z = 0 \) \( \mu \)m). Loading conditions are same to previous section but the magnitude of the pressure is changed to 1.0 GPa in the fatigue failure simulation. In addition, a 0.5\( \delta \) thickness no-fail zone is assigned on the bottom of the sample. See supplementary material for a movie showing the evolution of damage in the sample. Figure 14 shows damage maps and the corresponding microstructure of the back
surface \((Z = 0 \, \mu m)\). Boundaries of the sample are illustrated by lines. Damage results are consistent with strain results in Figure 5 because the model is linear elastic. Notice that most damaged nodes have damage index smaller than 0.05 throughout the evolution simulated in our fatigue tests. However, on some of the boundaries, we find locations with significantly larger damage index, near 0.35. These sites approach the development of a micro-crack. We can predict that cracks will develop from these sites, coalesce, and propagate along the twin grain boundary in the bulk which is already weakened by the existing damage. In addition, grain boundaries with high strain concentration have many damages material points. These grain boundary would be sources of cracks as observed in experiments.

![Damage maps and microstructure](image)

Figure 5.14: Damage maps (top row) at 0.02, 0.04, 0.06, 0.08 million cycles, and microstructure (bottom row) of the surface \((Z = 0 \, \mu m)\).

### 5.2 Conclusions

The peridynamic cubic elasticity model is used to study the strain concentration sites of a superalloy. Three verification case studies are performed: first, we test the effective modulus
along three group of directions by this cubic elasticity model, and compare results with theoretical values. The difference between simulated and theoretical values are decreased to 3% as horizon size decreases to $1.6 \, \mu m$. Second, averaged micromodulus are used to treat the interface issue in simulation, which is micromodulus of a bond crossing grain boundary depends on two different set of material properties. A two-grain model is used to show that the averaged micromoduli can provide desirable results. Again, smaller horizon size provides better match with the local method. Finally, we simulate a complex synthetic model of a Ni-based superalloy use the peridynamic cubic elastic model. Results show that most strain concentration appears at the twin grain boundaries. We compare simulation results with commercial finite element software ANSYS. Promising results are obtained, by comparing results on the surface and in the bulk of the sample between two methods, the peridynamic cubic elastic model provides almost identical strain distribution and strain concentration sites as ANSYS. Also, the peridynamic model captures strain concentration sites on triple grain junctions. A fatigue failure simulation is performed to show the capability of the current method, which shows that the peridynamic model can predict the crack nucleation sites in polycrystalline superalloy. Developing a peridynamic crystal plasticity model will be the future work.
Chapter 6 Future work

There are a few aspects of future work:

- Comparing with local methods, peridynamic simulation is computationally costly. Computational efficiency can be improved by using graded mesh like finite element method and variable horizon size. Using these two techniques, we can use much less number of the peridynamic nodes to perform the simulation, especially for structural components with holes and notches.

- Another option to improve the computational efficiency of peridynamic static simulation is using several models with different discretization density. The simulation starts from solving the coarse model with lease number of material points which requires, and then we can mapping the node displacement to a finer model. Repeat this procedure until desirable accuracy obtained.

- Fiber reinforced composites (FRC) are widely used in engineering because of its high strength at low weight. Failure in FRC is complex which includes inter-layer and intra-layer failure. Combining existing peridynamic FRC models with static and fatigue simulation discussed in this thesis, we expect to capture the complex failure phenomenon in in laminate materials.
6 Bibliography


[66] Q Le and F Bobaru. “Surface corrections in peridynamic models in elasticity and fracture”. In review.


[73] X Sun et al. “Intragranular particle residual stress strengthening of $\text{Al}_2\text{O}_3 - \text{SiC}$ nanocomposites”. In: *Journal of the American Ceramic Society* 88.6 (2005), pp. 1536–1543.


