



Uncovering the dynamic fracture behavior of PMMA with peridynamics: The importance of softening at the crack tip

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ABSTRACT

Recent experimental investigations of dynamic crack propagation in PMMA induced by impact show single cracks running stably at around 300–400 m/s. Existing numerical models for simulating dynamic fracture in PMMA consistently produce crack propagation speeds significantly higher than those measured experimentally. Here we uncover the reason for this puzzle by showing that localized material softening in the fracture process zone (caused by heating due to high strain rates in front of the crack tip), leads to crack propagation speeds that match the observed ones. We introduce a new constitutive model in our peridynamic formulation for PMMA to account for a softer material in the crack tip region. With the new model, the computed crack speed and crack length evolution match very closely those found experimentally.

1. Introduction

PMMA (polymethyl methacrylate) is a thermoplastic polymer used as an alternative to glass because of its transparency and low density. PMMA's dynamic fracture behavior make it widely used in many industries: automotive, aerospace, medical, etc. Dynamic fracture of monolithic and bi-layered PMMA samples using Digital Gradient Sensing (DGS) technique was recently studied in [1]. Crack propagation speeds for stable crack growth in the monolithic sample were found to be in the 300–400 m/s range. Other experimental studies reported similar crack speeds for stable crack propagation [2–4]. Cracks in PMMA can also grow unstably, in which case crack tip velocities reach higher values [5–7]. Some earlier works hypothesized a nonlinear process zone that could affect crack velocity [8,9].

Computational modeling of dynamic crack growth in PMMA has consistently shown much higher stable crack propagation speeds than those measured experimentally. The comparative simulation study in [10] showed faster crack speeds found by XFEM and element deletion technique than those measured. It was noted that when making the PMMA fracture energy five-six times higher than the actual one, the computed crack speed is reduced. Dynamic crack propagation in PMMA was also studied in [11] where the crack speed obtained using several computational methods (XFEM, peridynamics, cohesive zone model) were compared. Again, all of the methods utilized in [11] produced significantly higher crack propagation speeds than in experiments. In another recent paper [12], the dynamic crack speed was computed by an approach called bond-particle method (BPM). The BPM also leads to a computed crack speed from dynamic fracture in PMMA that is much higher speed than observed in experiments.

In this paper, we try to understand the reasons behind the failure of computational models in capturing the measured crack speed for dynamic fracture in PMMA. We first confirm that a peridynamic model utilizing a linear-elastic with brittle-failure leads to the faster-than-measured crack propagation speed in the impact and dynamic fracture in a monolithic PMMA sample tested

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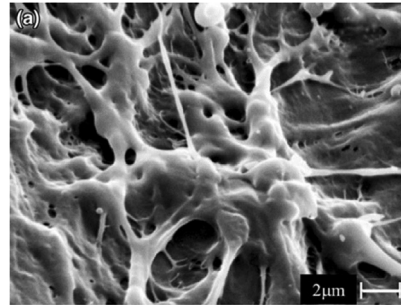


Fig. 1. SEM photomicrograph of PMMA fracture surface suggesting localized melting (from [14]).

experimentally in [1]. While the results, in terms of crack path and propagation speed converge in the limit of the horizon going to zero, the crack pattern is different from the one observed in experiments, and the discrepancy in the crack propagation speed is a factor of two. To remove some possible causes for this discrepancy and better understand the dynamic fracture in PMMA, we vary the impact loading for a possibly better match with the actual one. While this effort leads to a single straight crack path, as observed experimentally, it does not resolve the crack velocity problem as the computed crack still runs at almost twice the speed measured.

We hypothesize that PMMA's behavior at high strain rates (like those involved in the impact experiments in [1]) is different from the simple model used. Indeed, although similar to glass in some respects, PMMA has a very different microstructure compared to glass, featuring long chemical chains, cross-linked. Before fracture occurs, deformations of the polymer network can cause a measurable temperature rise. The localized heating ahead of the crack tip is caused by the fast straining of macromolecules in the fracture process zone [13]. PMMA's behavior under high strain rate impact by using a split Hopkinson pressure bar was studied in [14]. The SEM photomicrographs of fracture surfaces showed some local melting. For this to occur, the local temperature had to reach higher than the softening temperature of PMMA (see Fig. 1). The estimated maximum temperature generated at the crack tip was around 530 °C [14]. The temperature rise near the crack tip in PMMA was studied using temperature sensitive liquid crystal film and infrared detector in [15]. It was indicated that the rise of temperatures (around 500 K) at the crack tip in PMMA did not change much as the crack tip velocity varied between 200 m/s and 600 m/s (see Fig. 2).

Computational models utilizing local softening in simulating dynamic fracture in PMMA do not exist. Based on these observations, we introduce a new peridynamic constitutive model – bond force and bond strain relationship in peridynamic- that accounts for softening in the fracture process zone. This approach is meant to reflect the actual softening produced by the local heating that is triggered under the high strain rates present in the fracture process zone. We test the new model in terms of crack propagation speed to determine the appropriate size of the softened region. The peridynamic computations reveal a shift in the time scale from the moment of impact until the first data point reported in the experiment. When this time-shift is implemented, we find that the new model is able to explain the observed behavior. This peridynamic model is the first to validate experimental results on dynamic fracture in PMMA.

The paper is organized as follows: Section 2 presents a brief review of peridynamics; in Section 3 we describe briefly the PMMA impact experiment from [1], and experimental results that will be used for comparison with those from the peridynamic model; in Section 4 we discuss the loading conditions in detail with the help of a full 3D LS-Dyna simulation and show the discrepancies between the regular linear-elastic-brittle PD model and the experimental results; in Section 5 we introduce the new constitutive model that accounts for softening (induced by local heating) in the fracture process-zone and determine the appropriate size for the softened elastic zone; we present conclusions in Section 6.

2. A brief review of peridynamics

Peridynamics was introduced as a nonlocal form of continuum mechanics by Silling in 2000 [16] for modeling damage and fracture. Since then, it has been extended to a variety of other problems in which domain changes/discontinuities are part of the problem [17–22]. In this theory, each material point is connected through peridynamic bonds to other points within a certain neighborhood region called “the horizon region” [23]. The peridynamic bonds transfer forces/heat/mass between points and their

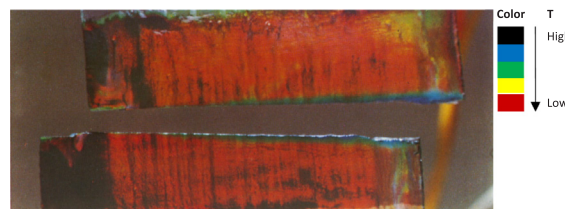


Fig. 2. Temperature rise along the crack path (left to right) measured by liquid crystal film (blue = higher temperature) (from [15]). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

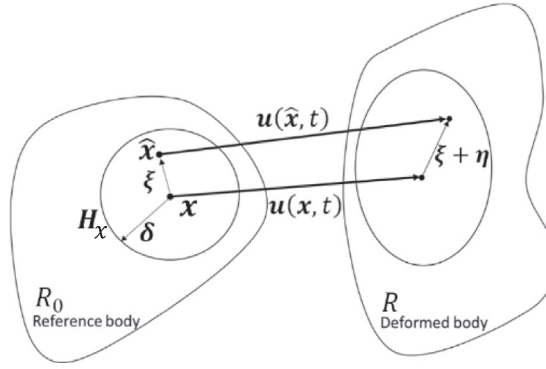


Fig. 3. The deformation of a peridynamic bond.

failure is used to define damage at a point. In peridynamics, one replaces the equation of motion by an integro-differential equation in which spatial derivatives are eliminated. This allows it to avoid the mathematical difficulties and inconsistencies present in the classical theory when cracks, for example, develop in the domain. The PD equations for dynamic problems are:

$$\rho \ddot{\mathbf{u}}(\mathbf{x}, t) = \int_{H_x} \mathbf{f}(\mathbf{u}(\hat{\mathbf{x}}, t) - \mathbf{u}(\mathbf{x}, t), \hat{\mathbf{x}} - \mathbf{x}) dA_{\hat{\mathbf{x}}} + \mathbf{b}(\mathbf{x}, t) \quad (1)$$

where $\ddot{\mathbf{u}}$ is the acceleration vector field, $\mathbf{u}$ is the displacement vector field as a function of point $\mathbf{x}$ and time t , $\mathbf{b}$ is the body force density, and ρ is the mass density. Also, $\mathbf{f}$ is the peridynamic pairwise force density function that describes the interaction between material points. The horizon region is the internal sub-region H_x (see Fig. 3), defined as:

$$H_x = \{\hat{\mathbf{x}} \in \mathcal{R}_0: \|\hat{\mathbf{x}} - \mathbf{x}\| < \delta\} \quad (2)$$

Let $\boldsymbol{\eta} = \mathbf{u}(\hat{\mathbf{x}}, t) - \mathbf{u}(\mathbf{x}, t)$ be the relative displacement and $\boldsymbol{\xi} = \hat{\mathbf{x}} - \mathbf{x}$ be the relative position in the reference configuration between two material points of $\hat{\mathbf{x}}$ and $\mathbf{x}$. From Eq. (2) we have $\|\boldsymbol{\xi}\| > \delta \Rightarrow \mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = 0$. When the pairwise force derives from a micro-elastic potential w , a micro-elastic material is defined by the following interaction force:

$$\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = \frac{\partial w(\boldsymbol{\eta}, \boldsymbol{\xi})}{\partial \boldsymbol{\eta}} \quad (3)$$

A linear micro-elastic material is obtained if we consider:

$$w(\boldsymbol{\eta}, \boldsymbol{\xi}) = \frac{c(\boldsymbol{\xi})s^2\|\boldsymbol{\xi}\|}{2} \quad (4)$$

where $c(\boldsymbol{\xi})$ is called the bond micromodulus function and s is the relative elongation of the bond, or the bond strain:

$$s = \frac{\|\boldsymbol{\eta} + \boldsymbol{\xi}\| - \|\boldsymbol{\xi}\|}{\|\boldsymbol{\xi}\|} \quad (5)$$

The pairwise force derived from Eqs. (3) and (4) is:

$$\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) = \begin{cases} \frac{\boldsymbol{\eta} + \boldsymbol{\xi}}{\|\boldsymbol{\eta} + \boldsymbol{\xi}\|} c(\boldsymbol{\xi}) s & \|\boldsymbol{\xi}\| \leq \delta \\ 0, & \|\boldsymbol{\xi}\| > \delta \end{cases} \quad (6)$$

This bond force-bond strain relationship can be viewed as the constitutive model in a PD formulation.

In this study, we use plane stress conditions, with the conical micromodulus choice (see [24]):

$$c(\boldsymbol{\xi}) = \frac{24E}{\pi\delta^3(1-\nu)} \left(1 - \frac{\|\boldsymbol{\xi}\|}{\delta}\right) \quad (7)$$

where E is the elastic Young's modulus, and $\nu = 1/3$ is the Poisson ratio in 2D plane stress conditions.

In peridynamics, damage is typically modeled using the critical bond strain concept, allowing a bond to break and no longer sustain a force [16,25] once its strain goes beyond a critical value. In this study, once a peridynamic bond breaks, it remains broken [17,18]. The critical bond strain parameter is obtained from the measured fracture energy, G_0 [25]. In 2D plane stress, the connection between s_0 and G_0 is [24]:

$$G_0 = 2 \int_0^\delta \int_z^\delta \int_0^{\cos^{-1}(z/\xi)} [c(\boldsymbol{\xi})s_0^2(\boldsymbol{\xi})/2] \xi d\theta d\xi dz \quad (8)$$

For the conical micromodulus given in Eq. (7), one obtains the critical strain as (see [26]):

$$s_0 = \sqrt{\frac{5\pi G_0}{9E\delta}} \quad (9)$$

The region defining the material is discretized with the one-point Gaussian quadrature, using uniform grid with spacing Δx (nodes are centered in the middle of each cell). The discretized (in space) version of Eq. (1), written at a time-step t_n is:

$$\rho \ddot{\mathbf{u}}_n = \sum_{j \in H_i} \mathbf{f}(\mathbf{x}_j, \mathbf{x}_i, t_n) V_j + \mathbf{b}_{i,n} \quad (10)$$

in which i , and j are node numbers, V_j is the volume of node j , and n is the time step number. For the temporal discretization we use the velocity-Verlet explicit scheme [27,28]:

$$\dot{\mathbf{u}}_{n+\frac{1}{2}} = \dot{\mathbf{u}}_n + \frac{\Delta t}{2} \ddot{\mathbf{u}}_n \quad (11a)$$

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \Delta t \dot{\mathbf{u}}_{n+\frac{1}{2}} \quad (11b)$$

$$\ddot{\mathbf{u}}_{n+1} = \ddot{\mathbf{u}}_{n+\frac{1}{2}} + \frac{\Delta t}{2} \ddot{\mathbf{u}}_{n+1} \quad (11c)$$

where $\mathbf{u}$, $\dot{\mathbf{u}}$ and, $\ddot{\mathbf{u}}$ denote displacement, velocity, and acceleration vectors, respectively.

Given that the uniform square discretization grid of the domain does not conform to the disk-shaped horizon region, several algorithms have been introduced to reduce the quadrature error caused by this [29]. The simple HHB algorithm (named so in [30] but introduced in [31]; see also [29]), provides monotonic convergence to the classical result, when the horizon factor increases. Here we use this algorithm, which corrects the bond length ξ for nodes that are only partially covered by the horizon region.

The nodal damage index is defined as the ratio of the number of broken bonds and the total number of bonds at that node. The value for the damage index varies between zero (intact material) and one (fully damaged). As we shall see below, in the new model it will be necessary to determine the position of the crack tip as the crack grows. We use a general algorithm that detects the crack tip based on the strain energy density value (see Section 5.1).

We use a PD code implemented to run on a single CPU with an NVIDIA Tesla P100 GPU [32]. The PD simulations using the smallest horizon (and densest grids) over 10 k time steps take about 10 min to complete on an Intel Xeon E5-2670 2.60-GHz processor with the Tesla P100 GPU.

3. Review of experimental test results

The dynamic fracture of monolithic and bi-layered PMMA samples using Digital Gradient Sensing (DGS) technique was studied in [1]. Here we only focus on the monolithic case. Material properties for PMMA are shown in Table 1. PMMA is a viscoelastic material and its elastic moduli increases at higher loading rates [33]. Under a high loading rate, polymer chains have lower molecular mobility and this leads to a higher Young's modulus [34]. The strain rate used in the experiments in [1] was around 25 s^{-1} . Because the fracture causing deformations analyzed in our study are induced by such rates, instead of using a more complicated strain-rate dependent model, for simplicity, we directly use the dynamic Young's modulus value of PMMA (see Table 1). This value is significantly higher than the static Young's modulus [1,33,35–39].

In the experiment, a rod was used as the striker, hitting a long bar which then transferred the loading into the PMMA via two inclined faces of a V-notch. The notch, at its end, has a 2 mm-long thinly cut pre-crack (by sharp razor blade). The crack path was recorded by 32 images which allowed for an estimation of the average crack propagation speeds. The dimensions of the PMMA specimen are illustrated in Fig. 4.a.

At the impact speeds used in [1], a single crack is observed to propagate through the monolithic sample in almost an straight-line fashion. Deviations from a straight-line crack trajectory (see Fig. 4b) could be due to small geometrical imperfections (leading to slight variations in wave reflections and interactions with the growing crack) or slightly asymmetric contact loading at the moment of impact. Histories of the experimentally measured (in [1]) crack tip velocity and crack length are shown in Fig. 5.

Table 1
Material properties for PMMA (from [1]).

	PMMA
Dynamic Young's Modulus, GPa	5.0
Poisson's ratio	0.34
Fracture Toughness, $\text{MPa}\cdot\text{m}^{0.5}$	1.31
Density, kg/m^3	1010
Thickness, mm	8.6

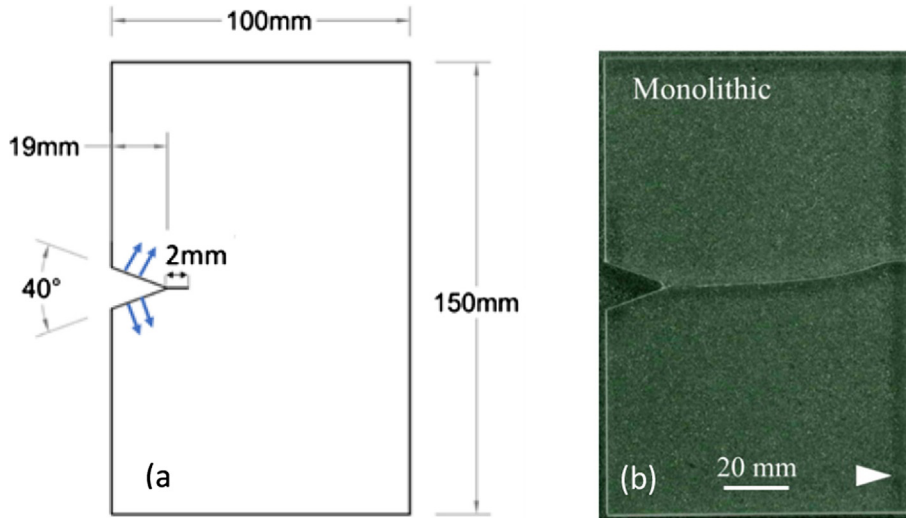


Fig. 4. (a) Geometry of the monolithic PMMA specimen used in [1]. Impact happens along the notch surfaces, and (b): Photograph of the fractured specimen showing crack path in a monolithic PMMA sample (from [1]). Arrowhead indicates crack growth direction.

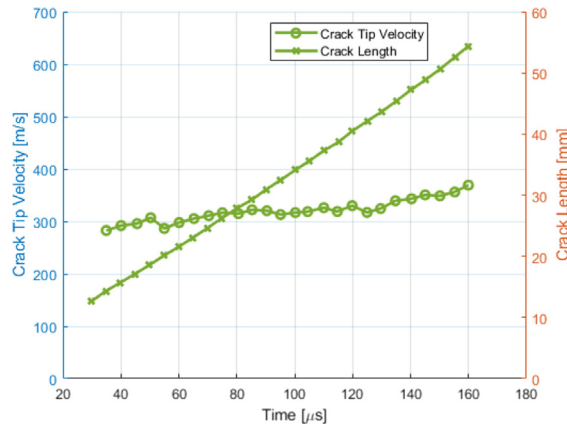


Fig. 5. Crack growth history from experiments (extracted and re-drawn from [1]).

4. Peridynamic modeling of the dynamic impact

4.1. Determining the loading conditions

Since the pressure pulse generated by the impact event was not reported in the experiments in [1], we setup a numerical model of the entire experiment including the contact between the bar and PMMA, to obtain an estimate of the loading conditions, in time, on the PMMA's V-notch. For efficiency, we create a 3-D finite element model in LS-DYNA to estimate this pressure pulse generated on the PMMA V-notch (see Fig. 6) before the fracture event. Although fracture in LS-DYNA can be simulated with the element deletion technique, for example, this approach is less accurate when the model geometry and inertia are important. Therefore, we will not model the fracture event in LS-DYNA, but instead use the pressure pulse from the finite element analysis as input data (applied body force) in the 2D PD simulation of the PMMA plate.

The PMMA has a pre-crack, and we define it in the LS-DYNA analysis by removing a tiny area with the length of 2 mm from the PMMA cross-section, before meshing. Calculated in this way, the pressure pulse will only be valid before fracture initiates in the sample [27]. Since the fracture initiation was not clearly defined in the experiment, we use the entire pressure pulse for our first PD simulation. Once we determine the fracture initiation time, t_f , (measured from the time of impact, the start of our PD simulation) from this PD simulation, we use the computed pressure pulse only up to t_f , and modify it after t_f (see Section 4.2).

The finite element (FE) model shown in Fig. 6 includes three parts, modeled as linear elastic materials a striker, a long bar, and a monolithic PMMA, all with the same dimensions as in the actual test in [1]. Element formulation #10 (tetrahedral) is used for the long bar and element formulation #1 (hexahedral) is used for the striker and PMMA. The long bar and striker are made of AL 7075-T6 with Young's modulus of 71.7 GPa. The PMMA material properties used are shown in Table 1. A single-surface contact is defined (coefficient of friction of 0.35) between the bar and the PMMA notch surfaces [35]. We apply the initial velocity of 15 m/s, used in

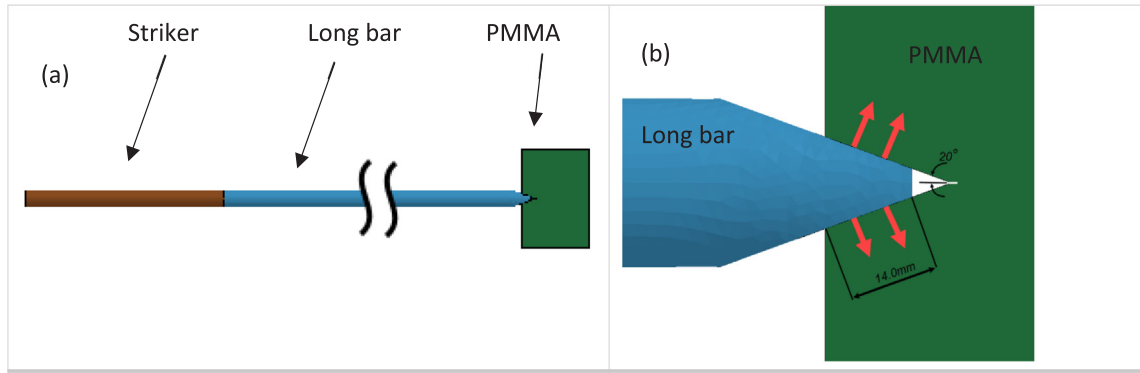


Fig. 6. (a) Geometrical setup in LS-DYNA FE model and (b) the interaction between the impacting long bar and the PMMA sample with the V-notch.

the experiment, on the striker part and we solve the FE model with the dynamic explicit solver [40]. This FE model has around 120 k nodes and roughly 350 k elements.

The resulting stress wave and its profile along the long bar are shown in Fig. 7.a and Fig. 7.b. The pressure pulse rises within 15 μ s, remains constant for about 100 μ s, and drops to zero after that. The average peak pressure is 106 MPa and matches the analytical calculation from $\sigma = 0.5\rho cv$, where c is the longitudinal wave speed, ρ is the material density, and v is the part velocity [41]. The compressive pressure on the V-notch is shown in Fig. 7.c. The pressure rises to 60 MPa within 60 μ s and drops after that. Since no fracture is modeled in LS-DYNA FE model, this load history is valid up to failure initiation in PMMA, which happens at t_f .

We consider a linear fit pressure profile as shown in Fig. 7.c, and then we convert it to the body force components. We apply this body force on the PD nodes located on parts of the V-notch surfaces (see Fig. 8 and [42]). It is important to notice that the impactor does not reach to the tip of the notch. We solve the 2-D bond-based PD model with stress-free boundary conditions on the remaining parts of the boundary.

4.2. Convergence study for dynamic fracture PMMA

We perform a δ -convergence study (horizon size decreases while keeping the number of nodes covered by a node's horizon roughly the same, see [43]) on the monolithic PMMA to see if the fracture patterns and crack speed converge. We use horizon sizes of 3.2, 1.6, and 0.8 mm with the horizon factor (the ratio of horizon size over the discretization size) of four.

Using the impact load shown in Fig. 7c, we calculate histories of crack tip velocities and damage maps with different horizon sizes shown in Fig. 9. Note that the fracture initiates at around $t_f = 20 \mu$ s from the time of impact (the start of the PD simulation) and the crack tip velocities found by the peridynamic model are approximately twice as fast as those measured experimentally. Interestingly,

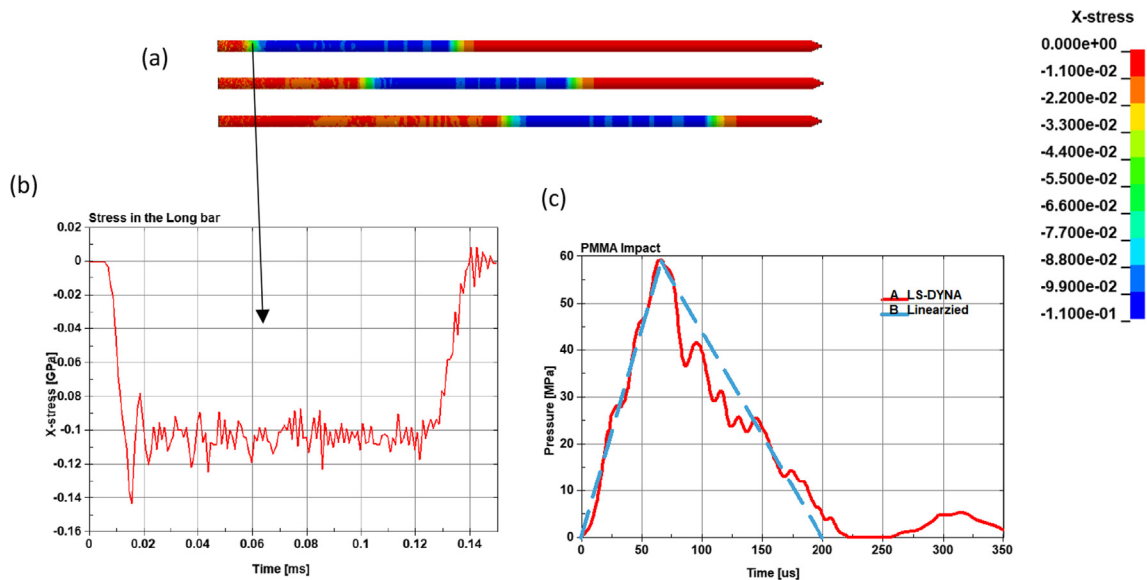


Fig. 7. (a) Compressive wave in the long bar, (b) the propagation of the compressive stress wave in the long bar, and (c) pressure measured on the V-notch surface.

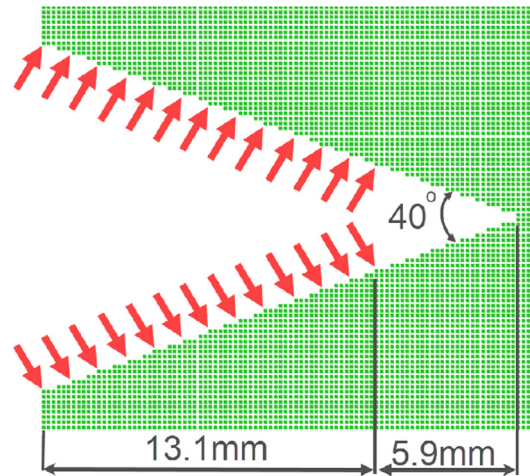


Fig. 8. The impact pressure from the bar is applied on PD nodes on parts of the V-notch surfaces as a body force.

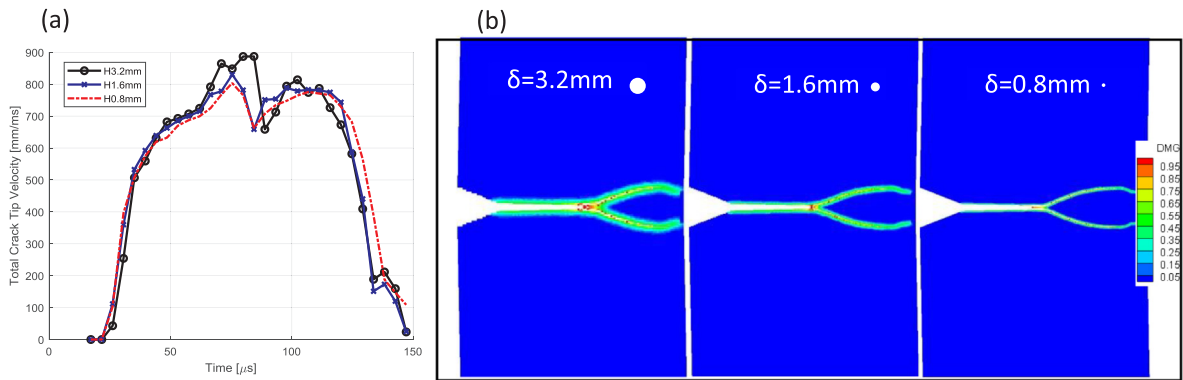


Fig. 9. Convergence study for the peridynamic model for the monolithic PMMA using horizon sizes of $\delta = 3.2$, 1.6, and 0.8 mm, respectively. (a) History of crack velocity and (b) deformed configuration at the end of the simulation. The colors show the damage distribution, and the small white disks show the relative size of each horizon region used. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

the crack in the monolithic PMMA branches, while the one in the experiment did not. In order to explain these discrepancies between the experimental observations and the results computed with the PD model, we offer two possible explanations: (1) Since the PMMA fractures at t_f (in the PD simulation), the pressure load (obtained by the FEM analysis) used after that is not valid and needs to be modified; and (2) dynamic fracture in PMMA could be influenced by factors like temperature rise at the crack tip that triggers softening in that region.

Using the pressure profile obtained from the LS-DYNA simulations before t_f , we test different possible load profiles (see Fig. 10). Keeping the load relatively constant for a duration of about 60 μs after crack initiation seems a good choice (see the behavior reported in a similar experiment in [44]). We investigate two possible unloading paths (see Fig. 10), since wave interactions can affect the crack propagation speed [45]:

- **Case I:** Applied pressure gradually drops to zero;
- **Case II:** Applied pressure suddenly drops to zero.

With both loading conditions (Case I and Case II) and a horizon size of 0.8 mm, the crack velocity (Fig. 10) oscillates before reaching values twice those measured experimentally in the monolithic sample (see Fig. 5). Note that, with the input loading shown in Fig. 10 for Case I, the crack path no longer branches and a single crack, fully splitting the sample, is obtained, as observed experimentally (see Video 1). For Case II loading, the crack arrests at 140 μs , and the sample is not fully split. The significantly faster computed crack propagation speed issue, however, is not resolved by only modifying the loading. Therefore, we test the second hypothesis, that the possible softening of the PMMA around the crack tip, caused by the local heating induced by high strain rates in the crack tip region (see Section 1), is responsible for the discrepancy between the computed and measured crack speeds.

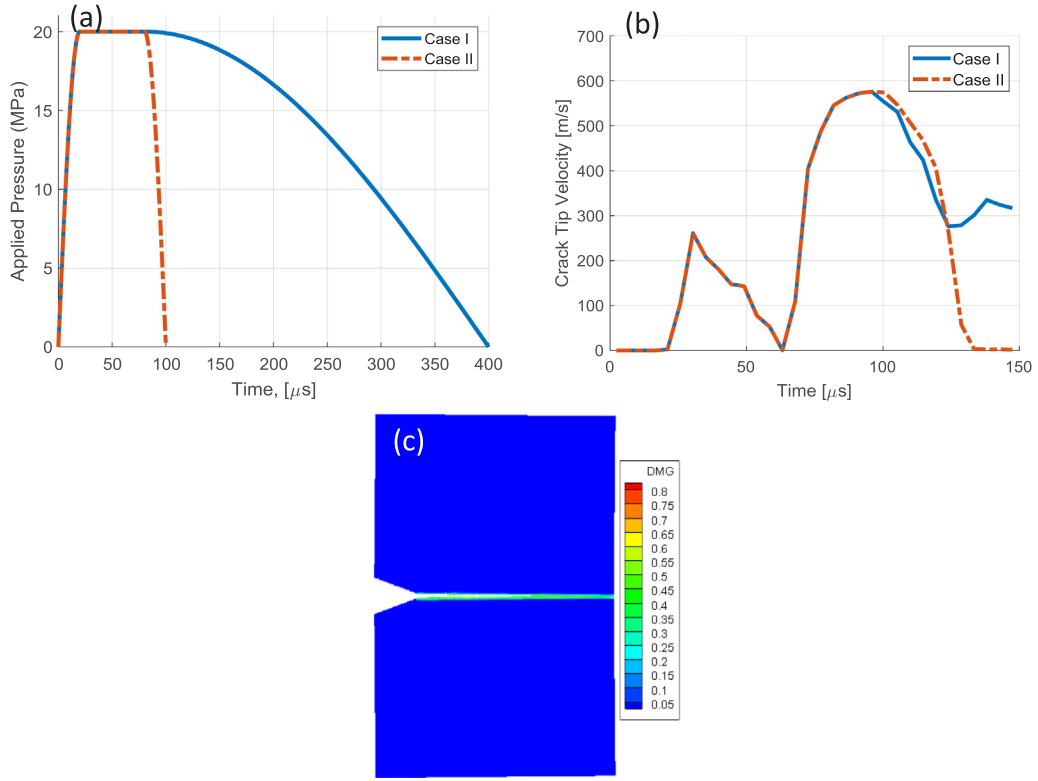


Fig. 10. Investigating load conditions with $\delta = 0.8$ mm. (a) two loading scenarios, (b) crack tip velocities for two loading cases, and (c) damage map and the crack trajectory for case I loading at $300 \mu\text{m}$ after impact (see also Video 1).

5. A new PD model accounting for softening due to heating near the crack tip

The other possible reason for which the PD results show crack speeds double those measured, is the presence of important temperature changes at the tip of the propagating crack and the subsequent softening of the material around the crack tip [15]. Temperature rise in dynamic fracture experiments in PMMA has been shown to extend of a thickness of around $3.0 \mu\text{m}$ into the banks of the crack [15,46]. Note that the size of the heated zone at the tip of the crack in PMMA is very small, therefore this type of fracture can still be considered as KI-controlled brittle fracture. In dynamic fracture of PMMA, most of the heat generated at the crack tip is caused by molecular scission, not by plastic deformation (see [13]). In this section, we test whether a brittle PD model that accounts for thermal softening near the tip leads to crack propagation speeds that match the experimental observations. We call the area in which we implement softening (by reducing the micromodulus values of bonds in this region) the “Heat Affected Zone” (HAZ).

5.1. Locating the heat affected zone around the crack tip

To apply the HAZ at the crack tip, we need to first determine the crack tip location ($\mathbf{x}_{\text{tip}}$) at each solution time-step (n). We use the strain energy density values (w_i^{n-1}) at each node x_i and time step ($n - 1$):

$$w_i^{n-1} = w(x_i; t_{n-1}) = \int_{H_{x_i}} w(\xi, \eta; t_{n-1}) \quad (12)$$

by using $w(\xi, \eta)$ for all unbroken bonds at step ($n - 1$) to locate $\mathbf{x}_{\text{tip}}$, defined here as the node with the highest strain energy density (see Fig. 11). After locating $\mathbf{x}_{\text{tip}}$, we check if a bond ξ is entirely inside the HAZ (if both of its end-nodes are inside the HAZ). For such bonds, we use a smaller micromodulus value, when their strain is a tenth of the critical bond-strain, resulting in a bi-linear force-strain elastic response. For all other bonds, the original linear model is used (see Eq. (6)).

As suggested in [9], we assume a circular shape for the HAZ with a radius r_{HAZ} (see Fig. 12). We define a parameter λ_{HAZ} that tracks whether a bond is inside the HAZ or not, based on the distances d_x and $d_{\hat{x}}$ of nodes $\mathbf{x}$ and $\hat{\mathbf{x}}$ to node $\mathbf{x}_{\text{tip}}$, as follows:

$$\lambda_{\text{HAZ}}(\mathbf{x}, \hat{\mathbf{x}}) = \begin{cases} 1, & d_x \leq r_{\text{HAZ}} \text{ and } d_{\hat{x}} \leq r_{\text{HAZ}} \\ 0, & \text{otherwise} \end{cases} \quad (13)$$

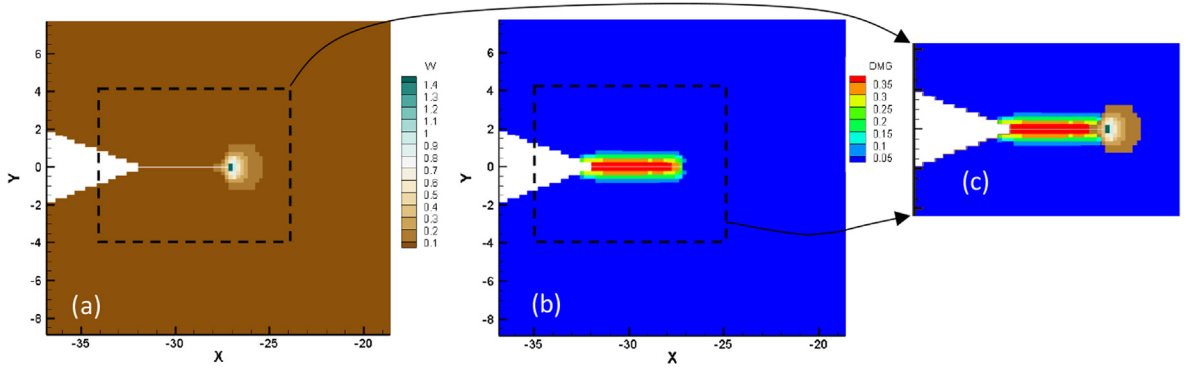


Fig. 11. Strain energy density (a) and damage index (b) in PMMA near the pre-crack tip. In (c), the superposed damage index and strain energy density maps, showing the location of the highest strain energy density in front of the crack tip.

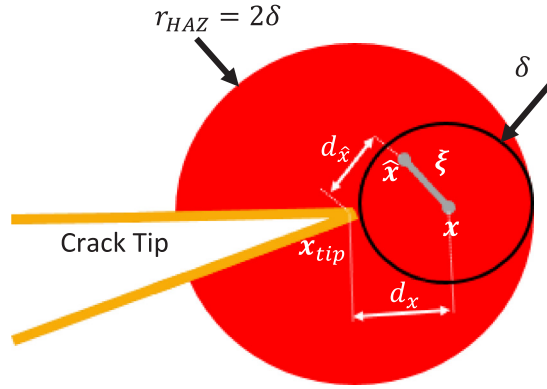


Fig. 12. Diagram for determining if a bond is inside the Heat Affected Zone (HAZ) for the case when its radius is 2 times the horizon size.

5.2. The new peridynamic constitutive model

As mentioned in the introduction, the temperature at the tip of a running crack in PMMA can be as high as 530 °C [14]. Experimental measurements ([35,47]) report that Young's modulus drops from 5.02 GPa at room temperature to 0.56 GPa at 659 K (see Table 2).

The fracture energy of PMMA appears to be independent of the temperature change (see [48]). Therefore, in this work we assume that the fracture energy does not depend on temperature directly. However, since the critical strain s_0 depends on Young's modulus value (Eq. (8)), and the modulus is significantly smaller in the HAZ, s_0 depends on location: the value in the HAZ is different from that in the rest of the sample. The new constitutive model, which takes into account the presence of the HAZ, for material inside the horizon of a given point, is set as follows (see Fig. 13):

$$f(\eta, \xi) = \begin{cases} \frac{\eta + \xi}{\|\eta + \xi\|} c(\xi) [0.1s + 0.09s_0], & \text{if } s > 0.1s_0 \text{ and } \lambda_{HAZ} = 1 \\ \frac{\eta + \xi}{\|\eta + \xi\|} c(\xi) s, & \text{otherwise} \end{cases} \quad (14)$$

Note that $f(\eta, \xi) = 0$ when $|\xi| > \delta$. We first assume the PD micromodulus is unchanged when the bond strain is smaller than $0.1s_0$ (see Fig. 13). However, if the bond is in the HAZ, as the overstressed macromolecules cause local heating, we decrease the micro-modulus to $0.1c$, according to the measured behavior in [13]. As observed experimentally, the crack runs fast from the beginning of its propagation. Therefore, we activate the HAZ from the onset of the crack growth and, keep it until the end of the simulation (see Fig. 5a).

To maintain the fracture energy G_0 constant, independent of whether bonds are in the HAZ or outside of it satisfied (areas under

Table 2

Young's modulus for PMMA at different temperatures (from [35,47]).

T (K)	200	250	300	350	400	450	500	550	600	650
E (GPa)	5.02	4.29	3.81	3.52	3.11	2.71	1.25	1.25	0.79	0.56

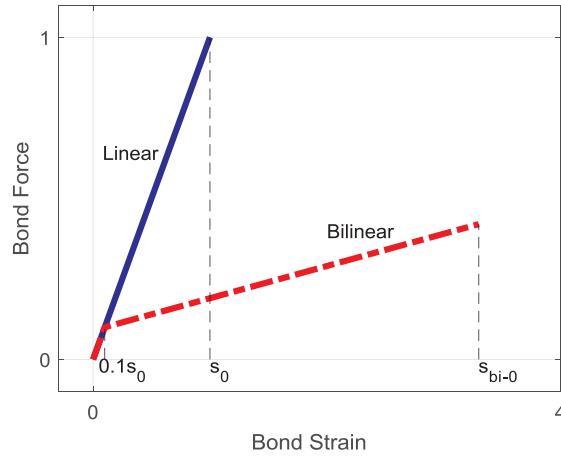


Fig. 13. Linear and nonlinear (bi-linear) bond force-strain relation for bonds outside and inside of the HAZ, respectively.

the bond force-strain relationships need to match), the following condition needs to be:

$$\frac{1}{2}cs_0^2 = \frac{1}{2}c(0.1s_0)^2 + c(0.1s_0)(s_{bi-0} - 0.1s_0) + \frac{1}{2}(0.1c)(s_{bi-0} - 0.1s_0)^2 \quad (15)$$

We find that the critical strain s_{bi-0} for the bilinear function needs to equal $2.40s_0$.

5.3. Determining the extent of the Heat-Affected-Zone

We now test the effect the HAZ extent has on our PD simulation results. Since the measured HAZ is much smaller than the horizon size used in this study, we calibrate the HAZ size by comparing the crack velocity with experimental data. One could use a model in which the horizon size is smaller than the measured heating zone, but that would lead to a much larger computational cost. Ways to reduce the cost of such computations could involve the coupling PD with FEM (see, e.g. [49]), but we do not pursue this here.

Because the starting time for the experimental data on crack length and velocity is not clearly identified in [1], we determine its relation to our computational starting time (the moment of impact) by placing the experimental data crack length values on the same graph with our computed values. We notice that a shift of about $90 \mu s$ in the time axis is required and we use the same time-shift for the velocity data (see Fig. 14).

Recall that with the original PD model (see Section 2), the crack tip reached velocities about twice the values measured in experiments (see Fig. 10b). With the new constitutive model, considering the HAZ near the crack tip, the crack tip velocity and the evolution of the crack length are shown in Fig. 14, together with the data from the experiment and the damage map at $400 \mu s$ after impact. Using a horizon size of 0.8 mm , three sizes for the radius of the HAZ are investigated with the **case I** loading (see Fig. 10a): δ , 2δ , and 3δ . As shown in Fig. 14a, the crack velocity is in the same range of values as the experimental ones only when the HAZ radius is larger than δ . Increasing the size of the HAZ from 2δ to 3δ does not change the crack speed by much. We can conclude that a HAZ radius of 2δ is a good choice for considering the effect of local heating in PMMA. Video 2 shows the dynamics of the crack growth.

Notice that the computed values for the crack propagation speed appear to be more oscillatory than those provided in [1], but, on average, the PD results match closely the measured speed values, and this is the reason why the evolution of the crack length matches

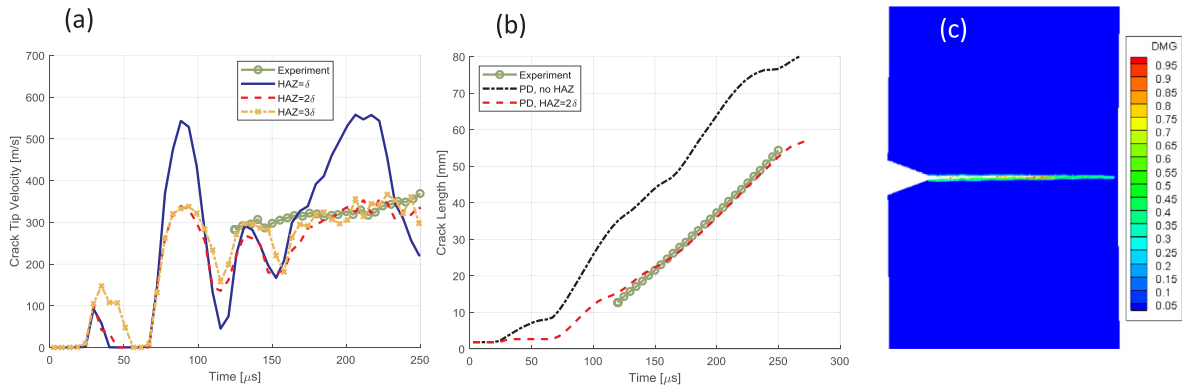


Fig. 14. Comparison between PD results and experiments: (a) crack speed for different HAZ values; (b) crack length with and without HAZ; (c) Damage map for HAZ = 2δ , at $400 \mu s$ after impact (see also Video 2). Experimental data taken from [1]. All results obtained using $\delta = 0.8 \text{ mm}$.

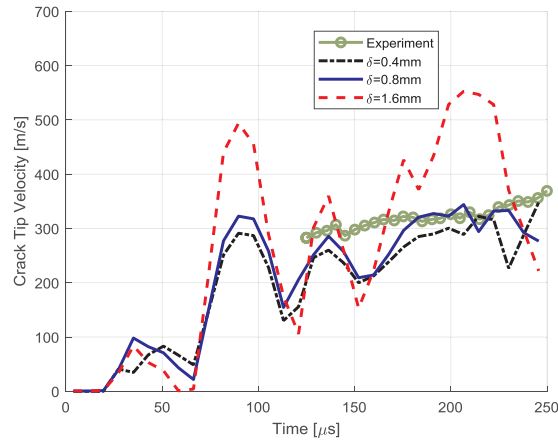


Fig. 15. History of the crack velocity in PMMA with horizon sizes of 1.6, 0.8, and 0.4 mm for a fixed HAZ radius of 1.6 mm.

very well with that provided in [1] (see Fig. 14). Crack speed fluctuations in the dynamic fracture of PMMA are not surprising: for example, in [5–7], dynamic instabilities are mentioned for crack propagation in PMMA when cracks reach speeds of 330 ± 20 m/s. Some of the oscillations seen in Fig. 14 might also be induced by the differences between the real loading profile and the one we used, and by the approximations we made in the constitutive model (no strain-rate dependence, approximate size of HAZ). The sensitivity of crack speed to loading is well-known ([45]). For example, we observe (see Appendix A) that by increasing the loading magnitude to reach a peak (at the same $t_f = 20$ μ s) that is 30% higher than case I loading, we find that the crack branches (the new PD model with HAZ is used) and the speed profile changes too (see Fig. 16).

We also evaluate the effect of decreasing the horizon size (and grid spacing) while keeping the HAZ size constant. We show the crack speeds for four horizon sizes (with the horizon factor of four) while HAZ size is fixed as 1.6 mm in Fig. 15. We observe that the crack velocity does not change much once the horizon size is less than half the size of the HAZ, and convergence is achieved.

6. Conclusions

In this paper, we found an explanation for a long-unanswered puzzle: the computed crack propagation speed in dynamic fracture of PMMA is significantly higher than that measured in experiments. It was observed that by using a regular linear-elastic-and-brittle-failure peridynamic model, the computed crack speed in PMMA is almost twice as fast as that measured experimentally. To explain the discrepancy, we hypothesized that material softening near the crack tip might be influencing the fracture behavior. Based on existing experimental evidence for temperature rise around the crack tip in dynamic fracture in PMMA, we considered a new model in which the effective Young's modulus is decreased significantly in the fracture process zone. We implemented a Heat Affected Zone (HAZ) around the crack tip in which a nonlinear (bilinear) elastic model is used before peridynamic bonds break. The model with a softened region around the crack tip reproduced the experimentally measured crack speed and the crack length evolution with high fidelity. The new peridynamic model allowed us to understand the relevant mechanisms in dynamic fracture of PMMA. With this model, we demonstrated the importance of the softened region around the crack tip in dynamic fracture of PMMA materials. The model will be used in the future to study the influence of strong and weak interfaces in bi-layered PMMA on crack behavior.

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Appendix A

In this appendix, we investigate the effect of load magnitude on the crack speed and fracture pattern/mechanism. A recent experiment on PMMA showed how sensitive the crack path is to the loading condition [50]. We increase by 30% the amplitude of Case I loading (see Fig. 10) and use PD with the HAZ (extent of the HAZ is 2δ) and the new constitutive model. The new impact load leads to a changed fracture pattern and a different crack speed profile (see Fig. 16). Interestingly, in this case, the crack branches early, whereas it did not branch with the lower impact loading.

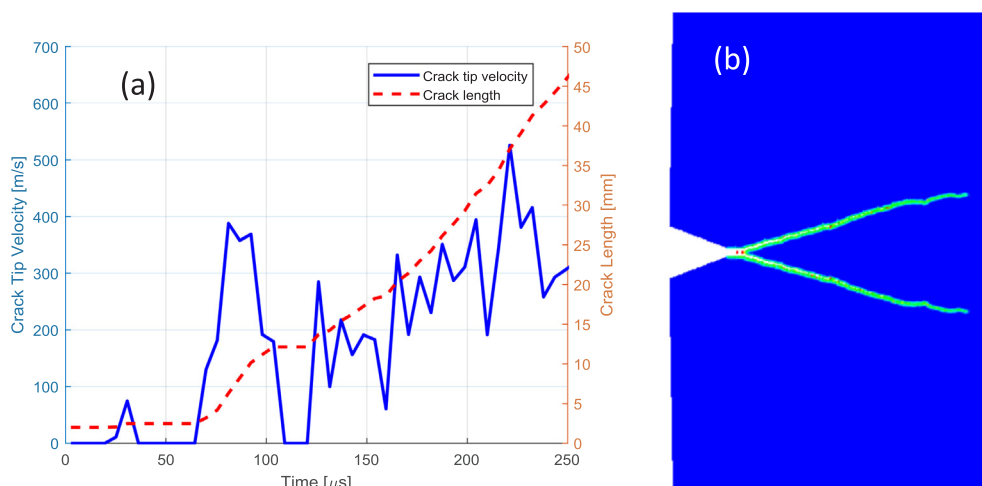


Fig. 16. A higher impact magnitude leads to crack branching near the pre-crack tip in the new PD model for PMMA that accounts for the softening due to heating. (a) Histories of crack tip velocity and crack length and (b) Damage map. Results computed using $\delta = 0.8$ mm.

Appendix B. Supplementary material

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.engfracmech.2019.106617>.

References

- [1] Sundaram BM, Tippur HV. Dynamic crack growth normal to an interface in bi-layered materials: an experimental study using digital gradient sensing technique. *Exp Mech* 2016;56(1):37–57.
- [2] Scheibert J, Guerra C, Celarie F, Dalmas D, Bonamy D. Brittle-quasibrittle transition in dynamic fracture: an energetic signature. *Phys Rev Lett* 2010;104(4):045501.
- [3] Guerra C, Scheibert J, Bonamy D, Dalmas D. Understanding fast macroscale fracture from microcrack post mortem patterns. *PNAS* 2012;109(2):390–4.
- [4] Gonzales OD, Luong K, Homma H, Eliasson V. Experimental investigation of dynamic fracture initiation in PMMA submerged in water. *J Dyn Behav M* 2016;2(3):391–8.
- [5] Sharon E, Fineberg J. Confirming the continuum theory of dynamic brittle fracture for fast cracks. *Nature* 1999;397(6717):333–5.
- [6] Fineberg J, Gross SP, Marder M, Swinney HL. Instability in dynamic fracture. *Phys Rev Lett* 1991;67(4):457–60.
- [7] Sharon E, Gross SP, Fineberg J. Local crack branching as a mechanism for instability in dynamic fracture. *Phys Rev Lett* 1995;74(25):5096–9.
- [8] Rosakis AJ. Analysis of the optical method of caustics for dynamic crack propagation. *Eng Fract Mech* 1980;13(2):331–47.
- [9] Theocaris PS. Local yielding around a crack tip in plexiglas. *J Appl Mech* 1970;37(2):409.
- [10] Song JH, Wang HW, Belytschko T. A comparative study on finite element methods for dynamic fracture. *Comput Mech* 2008;42(2):239–50.
- [11] Agwai A, Guven I, Madenci E. Predicting crack initiation and propagation using XFEM, CZM and peridynamics: a comparative study. *Proceedings 60th electronic components and technology conference (ECTC)*. 2010. p. 1178–85.
- [12] Kou MM, Lian YJ, Wang YT. Numerical investigations on crack propagation and crack branching in brittle solids under dynamic loading using bond-particle model. *Eng Fract Mech* 2019;212:41–56.
- [13] Basu S, Van der Giessen E. A thermo-mechanical study of mode I, small-scale yielding crack-tip fields in glassy polymers. *Int J Plast* 2002;18(10):1395–423.
- [14] Acharya S, Mukhopadhyay AK. High strain rate compressive behavior of PMMA. *Polym Bull* 2014;71(1):133–49.
- [15] Fuller K, Fox P, Field JE. The temperature rise at the tip of fast-moving cracks in glassy polymers. *Proc R Soc Lond A* 1975;341(1627):537–57.
- [16] Silling SA. Reformulation of elasticity theory for discontinuities and long-range forces. *J Mech Phys Solids* 2000;48(1):175–209.
- [17] Jafarzadeh S, Chen ZG, Bobaru F. Peridynamic modeling of intergranular corrosion damage. *J Electrochem Soc* 2018;165(7):C362–74.
- [18] Jafarzadeh S, Chen Z, Bobaru F. Peridynamic modeling of repassivation in pitting corrosion of stainless steel. *Corrosion* 2018;74(4):393–414.
- [19] Jafarzadeh S, Chen ZG, Zhao JM, Bobaru F. Pitting, lacy covers, and pit merger in stainless steel: 3D peridynamic models. *Corros Sci* 2019;150:17–31.
- [20] Bobaru F, Mehrmashhadi J, Chen Z, Niazi S. Intracply fracture in fiber-reinforced composites: a peridynamic analysis. *ASC 33rd annual technical conference & 18th US-Japan conference on composite materials*. 2018. p. 9.
- [21] Zhao JM, Chen ZG, Mehrmashhadi J, Bobaru F. Construction of a peridynamic model for transient advection-diffusion problems. *Int J Heat Mass Transf* 2018;126:1253–66.
- [22] Mehrmashhadi J, Chen Z, Zhao J, Bobaru F. A stochastically homogenized peridynamic model for intraply fracture in fiber-reinforced composites. *engrXiv* 2019. <https://doi.org/10.31224/osf.io/tymhs>. pp. 31.
- [23] Behzadinasab M, Vogler TJ, Peterson AM, Rahman R, Foster JT. Peridynamics modeling of a shock wave perturbation decay experiment in granular materials with intra-granular fracture. *J Dyn Behav M* 2018;4(4):529–42.
- [24] Ha Y, Bobaru F. Studies of dynamic crack propagation and crack branching with peridynamics. *Int J Fract* 2010;162(1–2):229–44.
- [25] Silling SA, Askari E. A meshfree method based on the peridynamic model of solid mechanics. *Comput Struct* 2005;83(17–18):1526–35.
- [26] Zhang G, Bobaru F. Modeling the evolution of fatigue failure with peridynamics. *Rom J Tech Sci Appl Mech* 2016;66:20–39.
- [27] Mehrmashhadi J, Tang Y, Zhao X, Xu Z, Pan JJ, Le QV, et al. The effect of solder joint microstructure on the drop test failure—a peridynamic analysis. *IEEE Trans Compon Packag Manuf Technol* 2019;9(1):58–71.
- [28] Mehrmashhadi J, Mallet P, Michel P, Termeyousefi A. Rapid fabrication of amphibious bus with low rollover risk: toward well-structured bus-boat using truck chassis. *Smart Struct Syst* 2019:1–8. (submitted for publication).
- [29] Bobaru F, Zhang G. Crack branching in dynamic brittle fracture. *Handbook of peridynamic modeling*. CRC Press, Taylor and Francis Group; 2016. p. 245–316.
- [30] Seleson P. Improved one-point quadrature algorithms for two-dimensional peridynamic models based on analytical calculations. *Comput Methods Appl Mech Eng* 2014;282:184–217.

- [31] Hu W, Ha Y, Bobaru F. Numerical integration in peridynamics Technical report Department of Engineering Mechanics, University of Nebraska-Lincoln; 2010
- [32] Abedini M, Akhlaghi E, Mehrmashhadi J, Mussa MH, Ansari M, Momeni T. Evaluation of concrete structures reinforced with fiber reinforced polymers bars: a review. *J Asian Sci Res* 2017;7(5):165–75.
- [33] Rosakis AJ. Analysis of the optical method of caustics for dynamic crack-propagation. *Eng Fract Mech* 1980;13(2):331–47.
- [34] Richeton J, Ahzi S, Vecchio K, Jiang F, Adharapurapu R. Influence of temperature and strain rate on the mechanical behavior of three amorphous polymers: characterization and modeling of the compressive yield stress. *Int J Solids Struct* 2006;43(7–8):2318–35.
- [35] Abdel-Wahab AA, Ataya S, Silberschmidt VV. Temperature-dependent mechanical behaviour of PMMA: experimental analysis and modelling. *Polym Test* 2017;58:86–95.
- [36] Raftopoulos D, Karapanos D, Theocaris P. Static and dynamic mechanical and optical behaviour of high polymers. *J Phys D Appl Phys* 1976;9(5):869.
- [37] Theocaris P. Static and dynamic stress intensity factors by the method of transmitted caustics. *J Eng Mater Technol* 1977:105.
- [38] Davies E, Hunter S. The dynamic compression testing of solids by the method of the split Hopkinson pressure bar. *J Mech Phys Solids* 1963;11(3):155–79.
- [39] Katsamanis F, Raftopoulos D, Theocaris P. The dependence of crack velocity on the critical stress in fracture. *Exp Mech* 1977;17(4):128–32.
- [40] Abedini M, Khlaghi EA, Mehrmashhadi J, Mussa MH, Ansari M, Momeni T. Large deflection behavior effect in reinforced concrete columns exposed to extreme dynamic loads. *engrXiv* 2019. <https://doi.org/10.31224/osf.io/6n5fs>. pp. 32.
- [41] Yu T, Qiu X. Introduction to impact dynamics. John Wiley & Sons; 2018.
- [42] Sundaram BM, Tippur HV. Dynamics of crack penetration vs. branching at a weak interface: an experimental study. *J Mech Phys Solids* 2016;96:312–32.
- [43] Chen Z, Niazi S, Zhang G, Bobaru F. Peridynamic functionally graded and porous materials: modeling fracture and damage. In: Voyiadis GZ, editor. *Handbook of nonlocal continuum mechanics for materials and structures* Springer International Publishing; 2017. p. 1–35. https://doi.org/10.1007/978-3-319-22977-5_36-1.
- [44] Dondeti S, Tippur HV. A hybrid experimental-numerical study of crack initiation and growth in transparent bilayers across a weak interface. *Conference proceedings of the society for experimental mechanics series*. 2019. p. 57–63.
- [45] Bobaru F, Zhang G. Why do cracks branch? A peridynamic investigation of dynamic brittle fracture. *Int J Fract* 2015;196(1–2):59–98.
- [46] Moy P, Gunnarsson CA, Weerasooriya T, Chen W. Stress-strain response of PMMA as a function of strain-rate and temperature. *Conference proceedings of the society for experimental mechanics series*, New York, NY, Dynamic behavior of materials, vol 1. 2011. p. 125–33.
- [47] Sahputra IH, Alexiadis A, Adams MJ. Temperature and configurational effects on the Young's modulus of poly (methyl methacrylate): a molecular dynamics study comparing the DREIDING, AMBER and OPLS force fields. *Mol Simulat* 2018;44(9):774–80.
- [48] Atkins AG, Lee C, Caddell RM. Time-temperature dependent fracture toughness of PMMA. *J Mater Sci* 1975;10(8):1381–93.
- [49] Galvanetto U, Mudric T, Shojaei A, Zaccariotto M. An effective way to couple FEM meshes and Peridynamics grids for the solution of static equilibrium problems. *Mech Res Commun* 2016;76:41–7.
- [50] Sundaram BM, Tippur HV. Dynamic penetration and bifurcation of a crack at an interface in a transparent bi-layer: effect of impact velocity. *Conference proceedings of the society for experimental mechanics series*, Cham, Dynamic behavior of materials. 2017. p. 69–74.