Microbranching in mode-I fracture using large scale simulations of amorphous and perturbed lattice models

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Abstract

We study the high-velocity regime mode-I fracture instability using large scale simulations. At large driving displacements, the pattern of a single, steady-state crack that propagates in the midline of the sample breaks down, and small microbranches start to appear near the main crack. Some of the features of those microbranches have been reproduced qualitatively in smaller scale studies on both a model of an amorphous materials (via the continuous random network model) and using perturbed lattice models. These previous studies (using $O(10^4)$ atoms) pointed to the need for performing larger scale simulations ($O(10^6)$ atoms), in order to achieve more physically realistic results. In this study, larger scale simulations were performed using multi-threading computing on a GPU device. First, we find that the microbranching pattern appears to be converging with the lattice width, i.e. the relative width of the microbranch region $\delta y/W$ decreases with increasing lattice width ($W$). This is a crucial test if the lattice simulations are to be used as an appropriate model for the experiments. Second, the microbranches using larger scale lattices yield sufficiently large microbranches as to enable a check of the statistics of the microbranches. The simulations reproduce the growth of the size of a microbranch as a function of the crack velocity, as well as the increase of the amplitude of the electrical resistance RMS as a function of the crack velocity. In addition, the simulations yield the correct branching angle of the microbranches, and the power law governing the shape of the microbranches seems to be lower than one, so that the side cracks turn over in the direction of propagation of the main crack as seen in experiment.

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I. INTRODUCTION

The study of the physics of brittle fracture has been very fruitful in the last two decades [1–3]. New experiments have shown various new features of dynamic fracture, focused in Mode-I (tensile) fracture using amorphous brittle materials [4–7]. In particular, the experiments have shown a sharp transition between the regime of steady-state cracks and the regime of unstable cracks [5–6]. In steady state, where the driving displacement, ∆ (of order ∆G, the Griffith criterion), is sufficiently small, a single crack propagates in the midline of the sample, reaching a steady-state velocity (which is of order the Rayleigh surface wave speed, cR). Increasing ∆ results in an increased steady-state velocity, yielding a v(∆) curve, until a specific critical point. Increasing the diving displacement further, beyond this critical point, we enter the unstable regime, where small microbranches start to appear nearby the main crack. The experiments have shown that above the critical point, the size of the average microbranch (which is log-normal distributed) increases rapidly with the crack velocity, measured via the slope of the electrical resistance of a conductive layer that is pasted on the sample. The electrical resistance slope exhibits oscillations whose amplitude increases rapidly as well. Increasing the driving displacement furthermore, the small microbranches become large microbranches, creating a complex fracture pattern, and finally, creates macrobranches [1–6] [8].

Some of the new experimental findings could not be explained via the classical theoretical approach for fracture mechanics, the linear elasticity fracture mechanics (LEFM) theory [9]. For example, several predictions of LEFM for the critical velocity, such as the studies of Yoffe [10] or Eshelby [11] predicted a single universal critical velocity much higher than that seen in some of the experimental studies, such as in PMMA [1]. Also, experiments have found various material-dependent features such as the terminal velocity which the crack manages to propagate as well as the critical velocity for macro-branches [1]. As far as the micro-branching critical velocity, the question of universality is debatable [12], but anyhow, the velocities are much smaller that the theoretical predictions. For a review, see the Introduction in [13]. However, the basic reason for the failures of LEFM is that the basic equations of LEFM yield a singularity of the stresses near the crack tip [9], and thus, the zone nearest to the crack’s tip (the process zone) cannot be modeled via LEFM.

The failure of LEFM, caused by this singularity, gave rise to an interest in discrete lattice
models and simulations [14][23]. In this kind of model, the basic length-scale which is the lattice scale, prevents the singularities that appear in the continuum approach. The lattice models were successful in reproducing the behavior of steady-state cracks [14][15][17], including a material dependency of the $v(\Delta)$ curves, in that it depends on the specific parameters of the inter-atomic potential [20][21]. In addition (concerning steady-state cracks), recently experiments in gels (that have three orders of magnitude slower sound speed than the classic brittle materials like PMMA or glass, which enables direct visualization by means of moderately fast video cameras) allows one to take clear snapshots of the crack tip [3][7][24]. We can see in Fig. 1 the excellent match of the crack’s tip shape between pure lattice simulations (described in detail below) and the experiments (for details, see the caption of Fig. 1). Moreover, the lattice models predict a certain critical point beyond which the steady-state solution becomes linearly unstable [18][21]. In the simulations, this is exactly the point which the crack stops propagating along the midline of the sample and some additional bonds, not along the midline, start to break [16][18][20][25]. However, especially in mode-I pure lattice simulations, the post-instability behavior of the lattice models do not match the experiments, neither qualitatively or quantitatively [20][25].

One recent approach to overcome these difficulties has been to turn to a more realistic model for an amorphous material, the continuous random network (CRN) model [26]. The continuous random network was suggested first by Zachariasen for describing amorphous material [27], and specific effective algorithms (using Monte-Carlo techniques) for generating the CRN were offered in [26][28][29]. Recent accurate 2D experiments using transmission electron microscopy (TEM) in 2D silica on the structure of this amorphous material were reproduced to excellent accuracy using the Zachariasen model [30][31]. After generating an amorphous CRN sample, molecular dynamics simulations were found to yield many of the important qualitative features of mode-I fracture experiments in amorphous brittle materials [26]. The simulations showed the birth of microbranches growing nearby the main crack, the increase of the size of the microbranches as a function of the driving displacement (or of course, the crack velocity), and the growth of the amplitude of the derivative of the electrical resistance with respect to the time as a function of the crack velocity.

Another direction recently examined was that of perturbed lattice models [13], which exhibited behavior similar to that of the CRN model, including the main features mentioned above. However, these simulations (both the CRN and the perturbed lattice simulations)
FIG. 1. (Color online) Several snapshots of the crack’s tip in steady-state mode-I fracture in experiments on gels. In the upper picture, when the crack length is small comparing to the sample’s width, the crack has the (well-known) parabolic shape. As the crack length grows, the finite size of the strip effects the crack’s tip shape, generating a “tadpole-like” shape. The lattice simulations reproduce the shape of the crack’s tip in the finite-size strip geometry. The simulations have (only) \(\approx 50,000\) atoms and thus, the results are scaled to the real size of the experimental sample. This “tadpole” shape is generic for finite-size (strip) lattice simulations, both honeycomb or hexagonal lattices with any amount of viscosity. Since the experimental crack is not exactly symmetric between the upper and the lower size of the crack, we used several values of \(\Delta/\Delta_G\) to get an optimal match between experiment and simulation (the small \(\Delta/\Delta_G\) shape is somewhat better on the upper side and the large \(\Delta/\Delta_G\) shape is somewhat better in the lower side). The experimental pictures are taken from [3].

suffered from a significant level of numerical noise, since each microbranch contained only a few tens of broken bonds at most. Thus, the statistics that concerns the most interesting physics, that of the branches, was quite poor.

These intriguing results, performed on limited size systems \((\mathcal{O}(5 \cdot 10^4)\) atoms) provide strong motivation to conduct larger simulations both to reduce the overall noise level and to get closer to at least a mesoscopic system where scaling behavior might set in. The goal was
to achieve at least a two magnitude increase in size, i.e., simulations of the order of millions of atoms \(\mathcal{O}(5 \cdot 10^6)\) atoms), which necessitated using parallel (multi-threading) computing. In this work we study mode-I fracture via large scale simulations, with a particular focus on the properties of the microbranches that could not be studied in the previous, limited size, studies.

The models are presented in Sec. II. In Sec. III we perform some basic checks of our models, confirming that the transverse size of the microbranch zone \(\delta y/w\) decreases with increasing sample width \(W\), for a given scaled driving displacement \(\Delta/\Delta G\) (in the experiments, using macroscopic sample sizes, the microbranching region width is much smaller than the sample width and the dynamics of the fracture is not effected by the sample edges). Next, in Sec. IV we present the quantitative results concerning the birth and the growth of the microbranches, and their physical features. A short discussion is presented in Sec. V.

### II. MODEL AND MAIN METHODOLOGY

The simulations presented in this study are divided generally into two kinds. The first one uses the continuous random network (CRN) model (to model an amorphous material), and the second employs a perturbed lattice model. Both models were described in depth in [26] and [13] respectively. We will review them here shortly.

#### 1. Generating the Continuous Random Network for modeling amorphous material

We generated two-dimensional CRN’s by a 2D-analogue [26] of the WWW algorithm [28, 29]. The potential that was used in the construction of the CRN included both a 2-body central force and a 3-body bond-bending force: [32, 33]:

\[
E_{\text{tot}} = \sum_{i=1}^{n} \left[ \sum_{j \in \mathcal{N}(i)} \frac{1}{4} k_r |\vec{r}_{ij}| - a_{i,j}^2 + \sum_{j,k \in \mathcal{N}(i)} \frac{1}{2} k_\theta (\cos \theta_{i,(j,k)} - \cos \theta_C)^2 \right],
\]

where \(|\vec{r}_{ij}|\) is the radial distance between each pair of nearest-neighbor atoms and \(a_{i,j} = a_0 = 4\) is a constant lattice scale (in contrast to the perturbed lattice model). \(k_r\) and \(k_\theta\) are the radial and the azimuthal (3-body) spring constants, respectively. \(\cos \theta_{i,(j,k)}\) is the cosine
of the angles between each set of 3 neighboring atoms, defined of course by:

$$\cos \theta_{i,j,k} = \frac{\vec{r}_{i,j} \cdot \vec{r}_{i,k}}{|\vec{r}_{i,j}| |\vec{r}_{i,k}|}$$  \hspace{1cm} (2)

where $i$ is the central atom and $(j, k)$ are its two neighbors. $\theta_C = \frac{2\pi}{3}$ (characterizing a honeycomb lattice). We start from a pure honeycomb lattice, randomize large number of bonds and perform a Monte-Carlo procedure, wherein each cycle we switch two bonds, calculating the optimal positions of the atoms in the near zone of the switched bonds to determine the change of energy so as to decide whether to accept the switch. Finally, we get a CRN that looks like Zachariasen’s patterns [26, 27] and the TEM snapshots of the 2D amorphous Silica [30, 31]. For a in-depth discussion, see [26].

2. Generating the perturbed lattice

Here we start with a perfect honeycomb lattice and randomize the lattice scale of each “bond”, $a_{i,j}$:

$$a_{i,j} = (1 + \epsilon_{i,j})a_0, \quad i = 1, 2, \ldots, n_{\text{atoms}}, j \in \mathcal{N}(i)$$  \hspace{1cm} (3)

where $\epsilon_{ij} \in [-b, b]$, and $b$ is constant for a given lattice, and in this work ranges between $0 \leq b \leq 0.1$, $a_0 = 4$. $\mathcal{N}(i)$ refers to the nearest-neighbors of site $i$. For a detailed discussion, see [13].

3. The equations of motion

In our model, between each two atoms there is a piece-wise linear radial force (2-body force law) of the form:

$$\vec{f}_{i,j} = k_r (|\vec{r}_{i,j}| - a_{i,j}) \theta_H (\varepsilon - |\vec{r}_{i,j}|) \hat{r}_{j,i},$$  \hspace{1cm} (4)

where the Heaviside step function $\theta_H$ guarantees that the force drops immediately to zero when the distance between two atoms $|\vec{r}_{i,j}|$ reaches a certain value $\varepsilon > a_{i,j}$ (the breaking of a “bond”). In this work we set $\varepsilon = a_0 + 1$. In addition there is a 3-body force law that depends on the cosine of each of the angles, acts on the central atom (atom $i$) of each angle,
and may be expressed as:

\[
\vec{f}_{i,j,k} \|= k_{\theta}(\cos \theta_{i,j,k} - \cos \theta_C) \frac{\partial \cos \theta_{i,j,k}}{\partial \vec{r}_{i,j,k}} \theta_H (\varepsilon - |\vec{r}_{i,j}|) \theta_H (\varepsilon - |\vec{r}_{i,k}|) \hat{r}_i = \] (5)

while the force that is applied on the other two atoms (atoms \( j,k \)) may expressed as:

\[
\vec{f}_{j,i,k} \|= k_{\theta}(\cos \theta_{i,j,k} - \cos \theta_C) \frac{\partial \cos \theta_{i,j,k}}{\partial \vec{r}_{i,j,k}} \theta_H (\varepsilon - |\vec{r}_{i,j}|) \theta_H (\varepsilon - |\vec{r}_{i,k}|) \hat{r}_j = \] (6)

Of course, the forces satisfy the relation: \( \vec{f}_{i,j,k} = - (\vec{f}_{j,i,k} + \vec{f}_{k,i,j}) \). In a honeycomb lattice there are three angles associated with each atom and in the hexagonal lattice there are six of them (we note that in the hexagonal lattice this choice is a little bit arbitrary since there are in general additional optional angles for each atom). There is a certain preferred angle \( \theta_C \) for which the 3-body force law vanishes (in the honeycomb lattice we set \( \theta_C = 2\pi/3 \) and in the hexagonal lattice we set \( \theta_C = \pi/3 \)).

In addition, it is convenient to add a small Kelvin-type viscoelastic force proportional to the relative velocity between the two atoms of the bond \( \vec{v}_{i,j} \): [17-20]

\[
\vec{g}_{i,j} = \eta(\vec{v}_{i,j} \cdot \hat{r}_{i,j}) \theta_H (\varepsilon - |\vec{r}_{i,j}|) \hat{r}_{i,j}, \] (7)

with \( \eta \) the viscosity parameter. The viscous force vanishes after the bond is broken. The imposition of a small amount of such a viscosity acts to stabilize the system and is especially useful in the relatively narrow systems simulated herein.

The set of equations of motion of each atom is then:

\[
m_i \ddot{\vec{r}}_i = \sum_{j \in 3p \, \text{nn}} (\vec{f}_{i,j} + \vec{g}_{i,j}) + \sum_{j,k \in 3p \, \text{nn}} \vec{f}_{i,j,k} + \sum_{j \in 6p \, \text{nn}} \vec{f}_{j,i,k}, \] (8)

In this work the units are chosen so that the radial spring constant \( k_r \) and the atoms mass \( m_i \) is unity.

After relaxing the initial lattice, we strain the lattice under a mode-I tensile loading with a given constant strain corresponding a given driving displacement \( \pm \Delta \) of the edges and seed the system with an initial crack. The crack then propagates via the same molecular dynamics Euler scheme using Eqs. [4-8].
4. Parallelization by GPU computing

As mentioned in the Introduction, the major innovation of this work, compared to our previous studies, is the use of large scale simulations. The previous studies of the amorphous (CRN) model [26] and the perturbed lattice model [13] used approximately 50,000 particles. In this study we wished to use approximately 5,000,000 particles. These kind of simulations cannot reasonably be performed by a single CPU, and thus force us to use multi-thread computing. We choose to use GPU computing, parallelizing the code via CUDA [34, 35]. This kind of programming forces the programmer to use the different levels of memory carefully [35], which makes possible achieving an acceleration up to \( \approx 100 \) faster than a regular C code using a single CPU. Beside the benefit of getting the results in a given system much faster, the main benefit is the possibility to run large scale simulations, which was prohibitive before. This tool makes possible the simulation of millions of atoms in reasonable simulation times.

Our model consists of several modules, each one of which needs to be re-written in CUDA. Both amorphous and lattice models use a molecular-dynamics module for the fracture simulations that must be parallelized. In addition, for the CRN, the Metropolis Monte-Carlo algorithm for generating the CRN needs to be parallelized. Furthermore, the electrical resistance simulations, which we use to determine the crack velocity [26], is solved by a nonlinear Laplace solver that needs to be parallelized too. In Appendix A we discuss briefly the degree of acceleration achieved for the different modules with the GPU using CUDA.

The various sized lattices we use contain:

- \( 162 \cdot 272 \approx 45,000 \) (\( N = 80 \) in the Slepyan model notation) atoms for the honeycomb lattice and \( 162 \cdot 408 \approx 65,000 \) atoms for the hexagonal lattice, which we call \( f = 1 \) (Factor=1). This size is equal to that used in our previous studies, [26] and [13].

- \( 486 \cdot 816 \approx 400,000 \) (\( N = 240 \) in the Slepyan model notation) atoms for the honeycomb lattice and \( 486 \cdot 1224 \approx 600,000 \) atoms for the hexagonal lattice, which we call \( f = 3 \) (Factor=3).

- \( 1458 \cdot 2448 \approx 3,600,000 \) (\( N = 720 \) in the Slepyan model notation) atoms for the honeycomb lattice and \( 1296 \cdot 3264 \approx 4,200,000 \) (\( N = 640 \) in the Slepyan model notation) atoms for the hexagonal lattice, which we call \( f = 9 \) (Factor=9).
In Appendix B we present a brief discussion regarding the results for the CRN using the parallel GPU Monte-Carlo algorithm. The GPU algorithm reproduced the results of the CPU code, in particular the agreement \cite{26} of the radial distribution function with that experimentally determined \cite{36} for amorphous silicon.

III. OVERVIEW OF THE SIMULATION RESULTS

In Figs. 2(a) to 2(c) we present the fracture pattern of the broken bonds for the small size perturbed honeycomb lattice (that was used before in \cite{13}, called here $f = 1$), for the intermediate size lattice ($f = 3$), and for the large lattice ($f = 9$), for three values of the driving displacement: small ($\Delta/\Delta_G = 2.8$), intermediate ($\Delta/\Delta_G = 3.4$), and large ($\Delta/\Delta_G = 4$). In the large driving simulation for $f = 1$ reported upon in our previous work, the microbranches reached the edge of the sample. In addition, in Fig. 3(a) we present fracture patterns using the amorphous CRN model (that was used before in \cite{26}) with $\Delta/\Delta_G = 3.6$ for the different sizes of lattices, and in Fig. 3(b), fracture patterns using a perturbed hexagonal lattice.

In the Figures we can immediately see the benefit of the larger scale simulations; the noisy fracture patterns that were obtained using $f = 1$ (the upper pattern in each figure), transform to the smoother and more physical-like patterns at $f = 9$. In Fig. 3(b) we can see clearly the curved power-law shape of the microbranches (for a quantitative discussion, see Sec. IV B).

A closer look reveals an important point: For a given driving displacement, the relative width of the fracture pattern decreases with the increase of the lattice size. This is crucial since otherwise the branching pattern in a macroscopic material would be macroscopic as well, against the evidence of the experiments \cite{5}. In Fig. 4, we can see the relative fracture zone width $\delta y/w$, when $\delta y$ is the width of the microbranching pattern, defined as the difference between the maximum and minimum $y$’s of broken bonds, and $W$ is the sample width. For any given value of $\Delta/\Delta_G$ the normalized width of the microbranching pattern decreases with the lattice width. This effect is seen clearly in the perturbed honeycomb lattice and in the CRN lattice, and in a more moderate way in the hexagonal perturbed lattice. This result is crucial; if the lattice models are physical, then when increasing the lattice size, the relative fracture zone must decrease, so that the branching does not remain macroscopic in
FIG. 2. (Color online) (a) The microbranching pattern in a perturbed honeycomb lattice for $\Delta/\Delta_G = 2.8$ and $\eta = 2$ for $f = 1$ in the upper curve, for $f = 3$ in the intermediate curve and for $f = 9$ in the lower curve. (b) The same for $\Delta/\Delta_G = 3.4$. (c) The same for $\Delta/\Delta_G = 4.0$.

the $N \to \infty$ limit, which would conflict with the experimental results).
IV. RESULTS

A. Length of microbranches

In this section we present the quantitative results for various features of the fracture patterns, especially the microbranches. First, we present the $v(\Delta)$ curve, the total amount of broken bonds in the microbranches, measured for a crack that reached the end of the strip, as a function of the crack velocity and the RMS of $dR(t)/dt$, the rate of increase of the electrical resistance as a function of the crack velocity. The results for the perturbed honeycomb lattice is presented in Fig. 5 and for the CRN in Fig. 6.

We can clearly see that in all three models the slope of the $v(\Delta)$ appears to saturate in the high velocity regime for the larger system sizes. This saturation is known from previous lattice studies [20]. The shape of the curves are similar to the experimental $v(\Delta)$ curves of real amorphous materials [1]. A close look at the curves of the total amount of broken bonds in the microbranches (which is our proxy for the average length of a microbranch
FIG. 4. (Color online) (a) The scaled width of the microbranching pattern $\delta y/W$ for (a) a honeycomb perturbed lattice, (b) the CRN model and (c) a hexagonal perturbed lattice, for different lattice sizes.

as measured experimentally, which we use to reduce the statistical noise) as a function of the crack velocity, using both the honeycomb perturbed lattice and the CRN, reveals quantitatively what we have seen qualitatively using small system sizes. Due to the noisiness of using finite size lattices, rather than two different regimes, with a single steady state crack at small velocities, and a sharp increase in the length of a microbranch in the large velocity regime, we get a smooth exponential behavior. However, the exponent of the curves increases robustly with the lattice size, sharpening the difference between the steady state regime and the microbranching (large velocity) regime. In addition we can see that in general, the CRN results act like a very perturbed honeycomb lattice, i.e., in any given $\Delta/\Delta G$, the number of broken bonds is larger in the CRN than in the perturbed honeycomb lattice, similar to what we saw in Ref. [13]. In addition, using the honeycomb perturbed lattice
FIG. 5. (Color online) (a) The $v(\Delta)$ curve of a perturbed honeycomb lattice using different lattice sizes. (b) Total number of broken bonds in the microbranches as a function of the crack velocity. (c) The RMS electrical resistance as a function of the crack velocity.

FIG. 6. (Color online) (a) The $v(\Delta)$ curve of a CRN lattice using different lattice sizes. (b) Total amount of broken bonds in microbranches as a function of the crack velocity. (c) The RMS electrical resistance as a function of the crack velocity.
FIG. 7. (Color online) (a) The $v(\Delta)$ curve of a perturbed hexagonal lattice using different lattice sizes. (b) Total size of broken bonds in microbranches, as a function of the crack velocity. (c) The RMS electrical resistance as a function of the crack velocity.

we can see the increase of the RMS amplitude of the derivative of the electrical resistance with respect to the time as a function of the crack velocity. At high velocities, the RMS amplitude is approximately three times greater than the amplitude in low crack velocities, in agreement with the experiments [5].

Looking at the results for the perturbed hexagonal lattice, we get one of the most important results of this paper. In Fig. 7(b), we present the normalized number of microbranches broken bonds (per number of bonds in the entire system) as a function of the crack velocity. The different curves (using various lattice size) are similar to each other, however, enlarging the lattice size, the transition become sharper with $f$. Using $f = 9$, we can see two different separate regimes (one of steady-state cracks, and one for microbranching), that looks very much alike the experimental result [5]. This result verifies the main assumption of the lattice models. The physical phenomena of microbranching is qualitatively described by lattice models and simulations, when enlarging the system size, the results become more quantitatively similar to the (macroscopic) experimental results.

B. Microbranching statistics

Having larger systems enables, for the first time, the generation of enough statistics to examine important quantitative features of the microbranches that have been measured experimentally [1, 5]. Since in this study, we obviously are restricted to 2D features only,
FIG. 8. (Color online) The distribution of the branching angle of the microbranches arise nearby the main crack using (a) a perturbed honeycomb lattice, (b) the CRN model and (c) a perturbed hexagonal lattice.

we focused here on the branching angle of the microbranches, and on the power-law shape of the microbranches.

The experimental studies on PMMA finds a narrow distribution of the branching angle between $20^\circ \leq \theta \leq 40^\circ$, with an average angle of $30^\circ$ [5]. We note that a previous study using a random perturbed Born-Maxwell model [37] yielded the wrong branching angle, namely $15^\circ$. In Fig. 8 we present the branching angle distribution of all the microbranches generated using all the values of $\Delta / \Delta_G$ in the different models that were used in this study. We can see that in all the models studied, the average branching angle is near $30^\circ$, very much like the experimental branching angle. The variance is different using the different models, where the variance of the CRN lattice is the narrowest, and thus most similar to the experiments.

One of the most striking features that was discovered in the experiments was a universal power-law shape of the branches, $y = ax^\alpha$, with a universal power, $\alpha \approx 0.7$ for several
FIG. 9. (Color online) The distribution of the power of the power-law shaping of the microbranches arise nearby the main crack using (a) a perturbed honeycomb lattice and (b) the CRN model.

FIG. 10. (Color online) (a) The distribution of $\alpha$, the power-law exponent ($y = ax^\alpha$) of the microbranches arising near the main crack for a perturbed hexagonal lattice. (b), A scatter-plot of the power $\alpha$ of the power-law exponent of the microbranches. We can clearly see that for the long branches, $\alpha$ converges on the value $\alpha \approx 0.7$, which is close to the experimental value.

different materials [11, 5]. On the one hand, our previous studies using CRN or a perturbed honeycomb lattice yielded only straight ($\alpha \approx 1$) microbranches [13, 26]. On the other hand, using a perturbed hexagonal lattice [13] we got branches that showed a power-law shape with $\alpha \approx 0.5$, though the results were noisy due to the relatively small number of broken bonds in each microbranch. We note also that the branches seen in the elastic beam model [38] or the Born-Maxwell model [37] look very noisy, without a clear power-law shape. In this study, using larger lattices we can check the shape of the microbranches based on relatively large microbranches ($\approx 100$ broken bonds in each microbranch). In Figs. 9 and 10(a) we can see the power distribution for the different kinds of lattices.
FIG. 11. (Color online) The distribution of $\alpha$, the power-law exponent ($y = ax^\alpha$) of the microbranches arising near the main crack for the perturbed hexagonal, perturbed honeycomb and CRN models, as a function of the micro branch length.

We can clearly see that the maxima of all the distributions are around $\alpha \approx 0.85 - 0.9$, which is indeed less than 1 (straight lines). Looking closely at the larger lattices ($f = 9$) in Figs. 2 and 3 we can see the nonlinear power law shape of the large branches, especially for the perturbed hexagonal lattice. In Fig. 10(b) we can see a scatter-plot of $\alpha$ as a function of the branch size for the perturbed hexagonal lattice case. It is clear that $\alpha$ converges on the value $\alpha \approx 0.7$ for the largest microbranches, which is close to the experimental value. The data for all three models is shown in Fig. 11. The other models do not show the decrease in $\alpha$ for the longest branches that is apparent for the hexagonal case, and perhaps data for longer microbranches are needed in the other cases, but in any case the asymptotic value of the exponent in all cases is less than unity.

V. DISCUSSION

We have used relatively large lattices fracture simulations using GPU parallel computing (with $O(5 \cdot 10^6)$ particles) for studying mode-I fracture. We find that the basic results from small lattices ($O(5 \cdot 10^4)$ particles) are confirmed using the larger size systems. The fracture patterns look more physical with a larger system, due to the large number of broken bonds in each microbranch. The width of the microbranch region relative to the system width decreases, a necessary condition if these models are to be taken seriously. The
basic properties of the microbranches, like the total length of the microbranches and the oscillations of the electrical resistance based velocity measurements, which were extremely noisy when using small lattices, look more smooth and realistic in the larger lattices. In particular there is now a clearer transition between the regime of steady state cracks, which there is a negligible amount of broken bonds beside the main crack, and the regime of instability, where the amount of broken bonds in the microbranches increases dramatically. The sharp transition is particularly clear in the hexagonal perturbed lattice (Fig. 7(b)).

In addition, important features of the microbranches that have been found and studied experimentally, are recovered in our large system simulations. The correct branching angle is found, and in the CRN lattice the correct variance is also obtained. The universal power-law shape that was found in different experimental studies [5] is recovered here, and for the larger branches, we get the correct power in the hexagonal perturbed lattice.

In future work, we plan to exploit the power of GPU parallel computing to run 3D simulations using \( O(5 \cdot 10^6) \) particles, with the goal of studying the different aspects concerning the 3D nature of the microbranches. We intend to check the similarities and the differences between 2D and 3D Mode-I fracture simulations, and to find the regime when the 2D model is sufficient, and on the other hand, the regime where 3D simulations are crucial.

Appendix A: GPU-accelerated C Code

In this appendix we discuss the run-times of the CUDA runs using a TESLA GPU for the different physical modules that were used in this study, and the acceleration ratios between a single CPU run and the GPU run. We re-wrote our C codes and replaced the main time-demanding functions by CUDA kernels [34]. We mention that we extensively employed the option of using shared memory to further accelerate the simulations, especially in the molecular-dynamics module [34, 35].

The parallelization of the main, molecular dynamics, module was to split the (potentially random, and thus general) grid of atoms to several physical zones; for the central elastic force law (and also for the viscoelastic force law) we sort the bonds and for the 3-body force law we sort the atoms. Each zone (“block” in the CUDA-jargon) loads the locations and the velocities to a fast shared memory, and each “thread” calculates the force of a certain bond (for the central force law), or atom (for the 3-body force law). Since the threads in
the same block execute simultaneously, we have to use CUDA Atomic commands to sum correctly the contribution of the forces acts from the neighboring atoms. Then, the new velocities and locations are calculated by simple CUDA kernels.

The electrical resistance module is basically solving a nonlinear Laplace equation. We used the methodology that was introduced in [39] for calculating the electrical resistance (a constant grid of bonds with $\sigma = 1$), while a cracked bond in the molecular-dynamics module determines the "cracked" ($\sigma = 0$) bonds in the constant grid of the electrical resistance. Thus, we used the same well-known methodology of using the CUDA kernels for solving 2D diffusion equations [35], including the use of shared memory. We implemented both Jacobi and red-black gauss-Seidel methods of solution, but no significant difference (in terms of the number of iterations for convergence) was found between the methods. In Fig. 12 we can see an example of the derivative of the electrical resistance with respect to the time using a perturbed honeycomb lattice for a specific $\Delta / \Delta_0$. We can see that using different size lattices (using the new GPU code in the larger lattices and the CPU code in the smaller lattice), we can see that the shape of the curves of electrical resistance look very much alike the experimental RMS amplitude of the crack velocity [5, 6] (that is measured via the electrical resistance [26]).

The parallel Monte-Carlo algorithm module for generating the CRN required extra care. Since each possible switch of bonds should be considered energetically independently, each switch should be separate from all the other simultaneous possible switches (to avoid overlapping of the switches and their neighboring zone). We mention that we use the parallel THRUST library (in CUDA) for sorting efficiently the nearest bonds for each bond, every given number of cycles.

In Figs. 13-14(a) we can see the typical run times for 1000 cycles (in seconds) for the molecular dynamics module and the Laplace solver module as a function of the system size. We can clearly see the benefit of using GPU computing, while the main benefit is the possibility to run systems with large number of atoms, which with a single CPU, was prohibitively time-consuming. The run-time using $\mathcal{O}(10^4)$ atoms with a single CPU is similar to the run-time using $\mathcal{O}(10^6)$ atoms with a single GPU. In Figs. 13-14(b) we see the acceleration ratios between a single CPU and a single GPU (of course, only for small systems, when a CPU run is available). We can see the significant acceleration, 40 times faster for the honeycomb lattice and over 50 times faster for a hexagonal lattice due to more demanding 3-body force
FIG. 12. (Color online) The derivative of the electrical resistance with respect to the time using a perturbed honeycomb lattice with $\Delta/\Delta_G = 3.4$ using the different lattice sizes. The plots are normalized in the $x$-axis to the $f = 1$ size (i.e. the $f = 9$ results are divided by 9 etc.)

FIG. 13. (Color online) (a) Simulation times (in [sec]) of 1000 cycles of the molecular-dynamics Euler scheme as a function of the system size (both using honeycomb and hexagonal lattices) using unoptimized $C$ code with CPU and with CUDA using GPU. (b) The acceleration run times between GPU and CPU as a function of the system size for honeycomb and hexagonal lattices.)
FIG. 14. (Color online) (a) Simulation times (in [sec]) for 1000 iterations of a Jacobi-method Laplace solver (for the electrical resistance) as a function of the system size using unoptimized C code with CPU and with CUDA using GPU (the times are similar also in Red-Black Gauss Seidel method). (b) The acceleration run times between GPU and CPU as a function of the system size.

FIG. 15. (Color online) (a) Simulation times (in [sec]) for a WWW Monte-Carlo scheme for producing a CRN (simulation stopped while the energy reaches half of the initial random energy) as a function of the system size using unoptimized C code with CPU, with CUDA using GPU and with the “old-CPU” code used in [26]. (b) The acceleration run times between GPU and CPU and the “old-CPU” codes as a function of the system size.

In the Laplace solver the speedup is a little bit lower and stands at approximately 25 times faster in GPU versus a single CPU.

In Fig. 15 we can see the run-times using a single CPU and the GPU. We can see here that the acceleration ratio here is lower then in the previous modules (about $\approx 5 - 10$), but still, in larger lattices (of $O(10^6)$ atoms), the benefit is clear. We mention that since the programming using CUDA is much more demanding from the programmer, especially
FIG. 16. (Color online) (a) The radial distance distribution of the bonds in CRN using different lattice size. (b) The angular distribution of the bonds in the CRN using different lattice size.

regarding the memory management, while re-programing the code, we improved our old-CPU code (that was in use in [26]), significantly; the acceleration ratio of the GPU code to the old CPU code is $\approx 60$.

Appendix B: CRN Monte-Carlo parallel CUDA algorithm

In previous work [26] we have shown that the CRN shares similar features with real amorphous matter, like amorphous silicon [36]. In this appendix we check explicitly the quality of the parallel GPU algorithm, generating a CRN. In Fig. 16 we can see the radial and angular distributions of the bonds in the CRN using different lattice size, and in Fig. 17 we can see the radial distribution function $g(r)$ using different lattice size. $f = 1$ (of $O(10^4)$ atoms) is the data using the old CPU code that was in use in [26], when larger lattices was produced via the new GPU algorithm.

We can see that the radial and angular distributions and the $g(r)$ curves are similar under the scaling of the lattice size (the number of the bonds or angles). This proves the validity of the parallel GPU algorithm, comparing the old CPU algorithm (that was verified before against experiments). Moreover, the RDF in the larger lattice size is smoother due to better statistics.
FIG. 17. (Color online) The radial distribution function (RDF or $g(r)$) of the CRN using different size of lattices.

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