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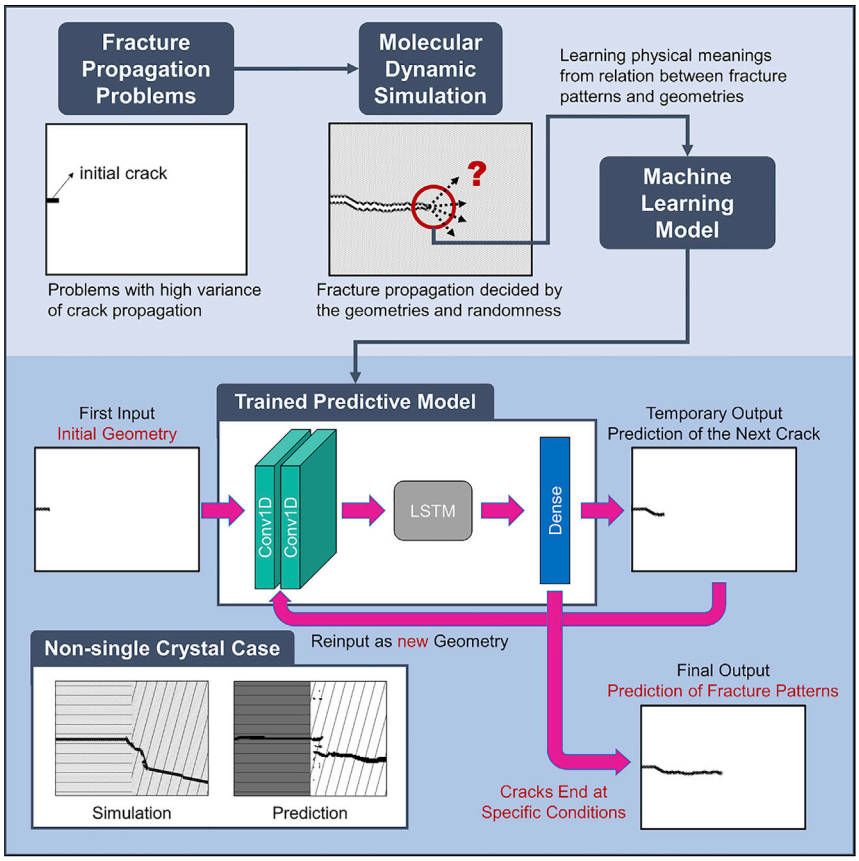
Using Deep Learning to Predict Fracture Patterns in Crystalline Solids



We use artificial intelligence (AI) to model the dynamic process of brittle fracture. This AI model enables us to evaluate the fracture toughness and dynamic fracture path efficiently as well as novel material microstructures. Scientists and engineers can now use this AI model as a powerful tool to design cutting-edge high-performance materials in a short amount of time.

Yu-Chuan Hsu, Chi-Hua Yu, Markus J. Buehler

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HIGHLIGHTS

The understanding of fracture process is critical for engineering materials

Fracture prediction in brittle materials is difficult

We present a machine-learning model to predict fracture processes in agreement with atomistic simulation results

Potential applications of this model include materials-by-design applications

3 **Understanding**
Dependency and conditional studies on material behavior

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Using Deep Learning to Predict Fracture Patterns in Crystalline Solids

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SUMMARY

Fracture is a catastrophic process whose understanding is critical for evaluating the integrity and sustainability of engineering materials. Here, we present a machine-learning approach to predict fracture processes connecting molecular simulation into a physics-based data-driven multiscale model. Based on atomistic modeling and a novel image-processing approach, we compile a comprehensive training dataset featuring fracture patterns and toughness values for different crystal orientations. Assessments of the predictive power of the machine-learning model shows excellent agreement not only regarding the computed fracture patterns but also the fracture toughness values and is examined for both mode I and mode II loading conditions. We further examine the ability of predicting fracture patterns in bicrystalline materials and material with gradients of microstructural crystal orientation. These results further underscore the excellent predictive power of our model. Potential applications of this model could be widely applied in material design.

INTRODUCTION

The ability to predict how cracks propagate in brittle materials is of great interest not only to scientific disciplines but also to developers of numerous technological applications.[1] Brittle fracture of solids has been widely studied using continuum mechanics modeling methods, such as extended finite approaches (e.g., extended finite element method [XFEM]),[2–4] phase field modeling,[5,6] cohesive zone modeling (CZM),[7] and many others, to estimate possible fragmentation patterns and fracture dynamics. However, dynamic crack propagation in brittle materials involves atomistic bond breaking, which often requires a thorough analysis using atomistic-level modeling,[8,9] which is rather difficult to address in continuum mechanics owing to the assumption of a continuum without the availability of details of chemical bond behavior.[10] Atomistic models, albeit sophisticated and predictive, are often computationally expensive and do not easily allow for rapid prediction of material performance. This hinders its effective application in material optimization, especially when considering the atomic scale as the fundamental design parameter. Here we propose a novel way to utilize data generated in predictive atomistic simulations to train a deep neural network, which allows us to make computationally efficient predictions.

Machine learning has drawn broad attention since the successes of deep reinforcement learning, such as evidenced in AlphaGo developed by DeepMind. In this work, the artificial intelligence (AI) model defeated top professional Go players.[11] Research efforts have also been devoted to understand physical problems, for instance, visualize the first image of black hole,[12] wave physics,[13] and protein folding.[14–17] The emergence of AI, mostly via machine-learning approaches, opens

Progress and Potential

Fracture is a catastrophic and complex process that involves various time and length scales. Scientists have devoted vast efforts toward understanding the underlying mechanisms for centuries, with much work left in terms of predictability of models and fundamental understanding. To this end, we present a machine-learning approach to predict fracture processes connecting molecular simulation into a physics-based artificial intelligence (AI) multiscale model. Our model exhibits predictive power not only regarding the computed fracture patterns but also for fracture toughness—the resistance of cracks to grow. The novel AI-based fracture predictor can also deal with complex loading conditions, here examined for both mode I (tensile) and mode II (shear). These results underscore the excellent predictive power of our model. Potential applications include the design of novel types of high-performance materials, composites design, surface coatings, or innovative bio-inspired structures.

a brand-new avenue for further research investigations. In particular, integrating machine learning and domain knowledge is critical to solving problems that have precluded efficient and scalable solutions (in many areas of biology, physics, and materials science).

AI can not only enable researches to expand the horizons of human knowledge but also solve problems with intractable numbers of combinations. In this context, materials scientists have applied machine learning to solve problems involving prediction of mechanical properties, design of structural materials, and improvement of simulation methods. Earlier works show that machine-learning models trained on the basis of datasets that capture material behaviors can be an efficient tool for prediction of mechanical behaviors, such as the Young's modulus of silicate glasses,[18,19] bulk moduli of metal-organic frameworks,[20] effective elastic properties of high-contrast composites,[21,22] and elastic deformation fields in a high-contrast two-phase composite system.[23–25] Other work in materials modeling and design has applied AI to design new composites, which can offer an efficient means to design and manufacture materials.[26–28]

These successful cases of adopting machine learning in varied research areas in the physical sciences typically result from the high efficiency and scalability of the approach. Previous studies especially related to fracture problems have applied machine learning to predict fracture paths by using a random forest method or convolutional-based models with data extracted from continuum levels.[29–31] However, we are currently lacking a machine-learning method to predict fracture mechanics that captures data sourced from the microscopic processes of bond breaking, derived from an atomistic point of view such as obtained from all-atom molecular simulations (e.g., molecular dynamics [MD]). However, the complexity of fracture mechanics predictions in traditional MD simulations with the high computational effort needed makes it difficult to provide results for materials design at the nanoscale. The work reported in this paper addresses this problem, and we anticipate that this method can indeed provide the capacity to perform atomic-level structural design for the next generation of materials. To solve the problem, we apply machine learning to learn fracture behavior of brittle materials through a special type of neural network composed of a convolutional neural network and a long short-term memory (LSTM) unit, a type of recurrent neural network.[32] Figure 1 provides a summary view of the method reported in this study.

In our machine-learning model, we adopt a convolutional LSTM (ConvLSTM)-based model[33–36] that is capable of learning the characteristics of spatiotemporal relations. This motivation is based on the fact that simulation results from MD contain a large number of atomistic information in time and space, reflected, for instance, in the dynamical evolution of fractures. In the ConvLSTM-based structure used here there are two kinds layers to capture distinct functions: The convolutional layer is capable of extracting features from images,[37,38] and LSTM is suitable for learning the connectivity of elements in a sequence. Motivating our work, there are several successful applications[39–41] in machine learning using ConvLSTM-based formulations that were used to learn and predict image-based sequences.

In MD, fracture propagation is often considered a highly stochastic problem because not only the geometry but also the random state of atoms will affect the simulation results of fracture problems. However, these two factors are high-dimensional so that their relations with the specific features of fracturing of interest for materials performance (such as fracture path or toughness) are too complicated to describe

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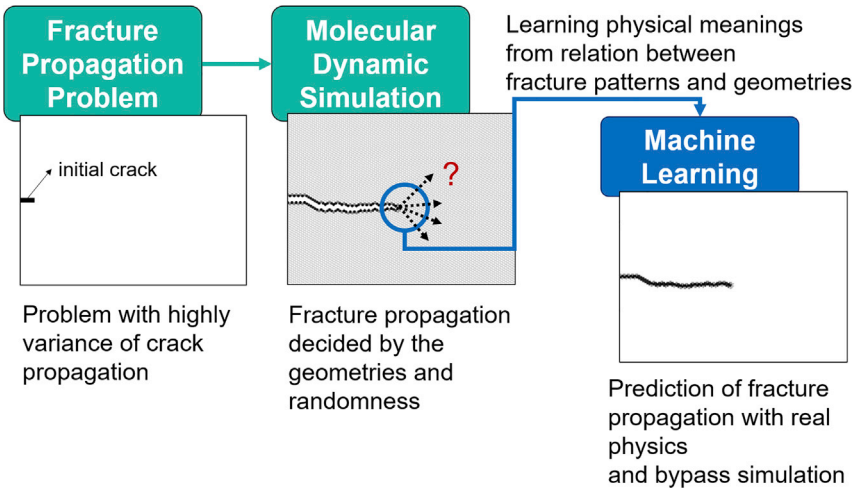

Figure 1. Overview of the Work Reported in This Paper

We propose a *de novo* approach to study the fracture problem with the crack patterns and crack length, based on a training set derived from molecular dynamics (MD) simulations. Our ultimate goal is to replace the stochastic problem of fracture propagation in MD simulations through a machine-learning model that can predict the overall crack propagation pathways. With our predictive machine-learning model, we realized an efficient way to explore the problem of fracture propagation bypassing time-consuming MD simulation, opening novel avenues for materials design solutions with atomistic-level degrees of freedom.

directly in a numerical approach. Hence, to create a dataset that contains rich enough physical embeddings for studying implicit relations between crack propagation and crystalline orientations, we conduct a large number of MD simulations of tensile tests of brittle materials with different crystal orientations. We then use several novel processing steps to properly represent the intrinsic physics of the MD simulation results in the image representation that is used in our machine-learning model. During this data processing, we translate the simulation results into a set of matrices. We then apply a ConvLSTM-based model to assess subtle changes in the fracture features of these MD simulation results.

The plan of the paper is as follows. We begin with a description of the molecular simulation of brittle materials (with a given molecular modeling force field and loading conditions), used here to develop a training set for our deep neural network. We then provide a detailed description of our deep neural network model and the preparation of the data as the training set. We further present an analysis of the training accuracy with 10-fold validation and confirm the capability of prediction for mode I and mode II fracture scenarios. We then use our machine-learning model to predict the fracture patterns in bicrystal materials and a sample of gradient orientation, which were not included in our training dataset. We conclude the paper with a discussion of future directions and concluding remarks.

RESULTS

Implementation of our deep-learning model is based on the concept of processing consecutive images as time sequences using convolutional LSTM layers, reflecting the patterns of crack spreads in different crystalline orientation as distinctive features. The training dataset was prepared from collecting fracture patterns from MD simulations. We then train the deep-learning model with this representation (for details see Experimental Procedures). Once the deep neural network is trained we can use it to predict crack patterns, whereby different crystalline orientations and

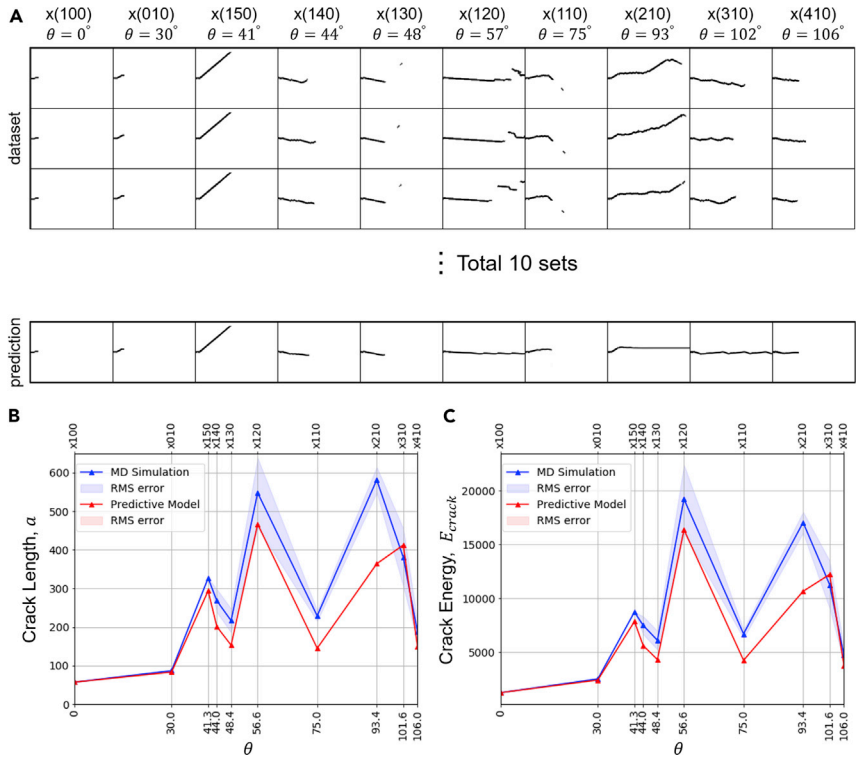

Figure 2. Results of Physics-Based Simulations of Tensile-Loaded Mode I Fracture Learned by Our Machine-Learning Model

(A) Dataset for the machine-learning model and predictions of single-crystalline orientation at specific strain. See also Video S1.

(B) Comparison of crack length between simulations and our predictive model.

(C) Comparison of energy release due to bond breaking between simulations and our predictive model.

an initial crack are used as a primer condition in each prediction scenario. We first vary the crystalline orientation to test the accuracy of our deep-learning model and then move on to predictions and validations of more complex scenarios.

Machine-Learning Prediction and Fracture Mechanics Study Validated by MD

The dataset of the crack patterns under 3.375% strain in mode I and the predicted results are shown in Figure 2A (the videos of predictions are shown in Videos S1I–S1X). The input of each case of prediction contains only the first 16 columns of the geometric matrix that includes the entire initial crack. We note that the strain in the simulation results used for the machine-learning model is free to choose in our method. The flexibility also means that the physical meanings that could be revealed by the machine-learning model are strongly related to the training set. In the simulation results of tensile test, the mechanical-energy-release rate varied in the same lattice but with different orientations due to the efficiency of loading for bond breaking.[42] The corresponding crack lengths are then calculated from the crack patterns in the crack images, pixel by pixel. As can be seen in Figure 2B, we compare crack lengths pixelwise in different orientations between images from MD simulation results and our predictive model. The predictions present similar variation of crack lengths in different orientations as MD simulations, which indicates that our model is not only sensitive to the difference in orientations but has also learned the implicit physical meanings of strain in crack images. This is an important result that indicates a level of generality and predictability in the results.

To further examine the reliability of our model, we pay close attention to the fracture toughness values[43] obtained from the MD simulations compared with the predictive model. To translate the physical meanings in the crack length to the fracture toughness in brittle materials, we first adopt Equation 1 to calculate the surface energy in MD simulations, where σ_{max}^2 is the maximum stress, E is the Young's modulus, and a_0 is the initial crack length (10 unit-distances in this study). The surface energy γ can be considered as a measure to determine how easily the fracture will propagate:

$$\gamma = \frac{\pi \sigma_{max}^2 a_0}{2E}. \quad \text{(Equation 1)}$$

We then adopt Equation 2 to calculate the energy loss by bond-break from MD simulations and predictions, where γ is the surface energy calculated from MD simulations, a is the crack length, and B is the thickness (where $B = 1$ in 2D materials):

$$E_{crack} = 2\gamma aB. \quad \text{(Equation 2)}$$

In Figure 2C, a comparison of energies from MD simulations with the prediction from our machine-learning model is depicted. The analysis shows that our framework is capable of effectively learning the real physical behavior and making excellent predictions.

To further examine the generality of the approach proposed here, we introduce another application of our machine-learning model for mode II fracture simulations, also in different crystalline orientations. For these cases, we build a second model identical in formulation to the model build for mode I, but trained against new data. Hence the dataset is replaced with crack images from mode II simulation results. The predicted results of the crack patterns are shown in Figure 3A. A further comparison of crack length and the crack energy is shown in Figures 3B and 3C. All predictions match well with the simulation results, except for the x100 case. We believe that the main reason why our machine model predicts non-stopping cracks for the x100 orientation is that cracks in that case only possess a simple horizontal pattern (in the direction of the initial crack position). To improve the predictive ability for the cases like the x100 orientation we might need more data, or information from other fields such as stress/strain distributions, to realize a more comprehensive model. The results still show that our model properly predicts the trend of crack propagation for most orientations, which shows the flexibility of our model to handle other, more complex, boundary conditions.

Overall Fracture Prediction of Bicrystal Case and Gradient Crystal Case

To explore other applications of our method for physical cases that were not included in the training set, we turn to study the overall fracture patterns that include initial cracks and branching behaviors, using a similar ConvLSTM-based structure by substituting the crack images of overall fracture for the training set. Furthermore, we can directly modify the geometric matrix input to make a prediction of more complex crystalline geometries. Here, we present two cases of bicrystal fracture predictions compared with MD simulation results. First, the prediction of a bicrystal case with small difference in orientations is shown in Figure 4A (the video of prediction is shown in Video S2A). Our model predicts that the crack patterns do not significantly change near the boundary, which is in good agreement with what we expected to see.

Another case with a larger difference in orientations of bicrystal material is shown in Figure 4B (Video S2B). In the MD simulation, the main crack first grows smoothly and horizontally, but turns at a large angle downward near the boundary. It then makes

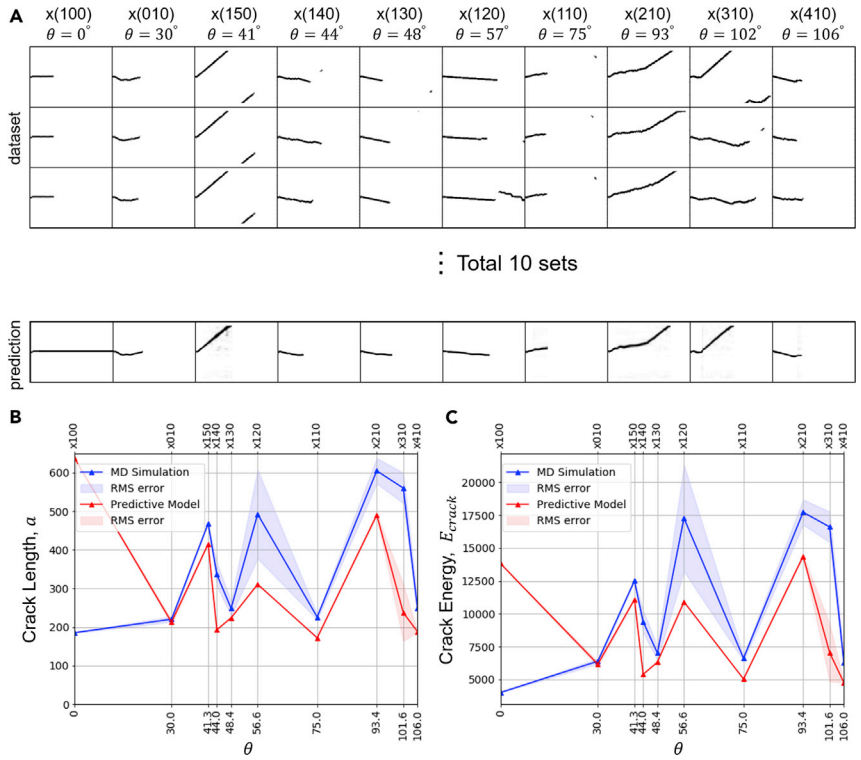

Figure 3. Results of Physics-Based Simulations of Shear-Loaded Mode II Fracture Learned by Our Machine-Learning Model

(A) Dataset for the machine-learning model and predictions of single-crystalline orientation at specific strain.

(B) Comparison of crack length between simulations and our predictive model.

(C) Comparison of energy release due to bond breaking between simulations and our predictive model.

another turn and propagates until overall fracture has occurred. Our model makes an acceptable prediction while the crack first starts to grow, in agreement with the MD simulation. One difference is that our model predicts a certain level of jagged patterns after the crack passes through the boundary, then turns the similar position of crack as does the MD simulation. Overall, the twisted crack patterns predicted by our model capture the behavior of crack propagation, albeit some details are not captured quantitatively.

Even if geometric conditions become more complicated, for example in gradient materials with continuously varying crystal orientations, we can use the model to make predictions outside of what was included in the training set. These predictions are made simply by continuously modifying the image-based geometric matrix input, as shown in Figure 4C (the video of prediction is shown in Video S3). The gradient crystal case shows us the potential of this method to make prediction on arbitrary geometry, bypassing MD simulations or complementing such approaches.

It is worth nothing that the additional scenarios discussed in the last few paragraphs are based on a model that has only learned from single-crystal simulations. Still, it possesses enough predictive power to make a solid prediction for bicrystalline cases as well as gradients of crystal orientations. When cracks come close to boundaries, our model creates some noise during the passing of the interface. This is likely because we have not fed our

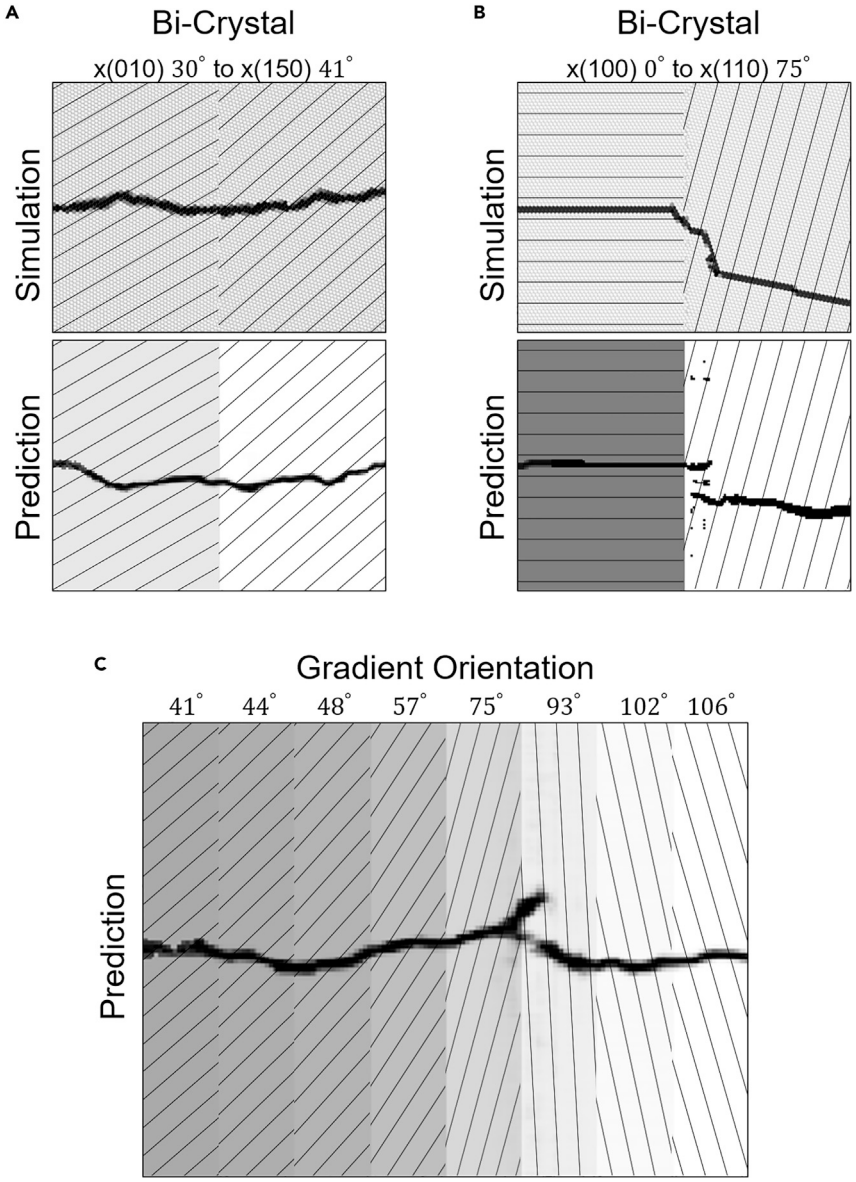

Figure 4. Additional Test Cases to Test the Predictive Power of Our Machine-Learning Model, Assessing Results for Cases that Were Not Part of the Training Set

Here we substitute the crack images of overall fracture for the dataset for machine learning.
(A) Prediction of overall fracture of small-difference bicrystal material.
(B) Prediction of overall fracture of big-difference bicrystal material.
(C) Prediction of overall fracture of gradient crystal material (such a system could be subject to optimization, e.g., to maximize fracture toughness or crack path tortuosity).

predictive model with the data involving the information of cracks near boundaries. However, once the crack leaves the unrecognized zone, the model immediately regains quantitative predictive ability. In short, it is perceivable that the predictive ability of this model can be further improved to address more complicated geometries if we add data related to simulation of complicated cases such as simulation results of bicrystal and gradient cases that include the crack patterns near boundaries. Also, there is a high chance of applying this approach to other numerical methods if the simulations results can similarly be mapped into the image-based matrices as proposed here. In conclusion,

machine learning in cooperation with image-based data representation for real physics opens up a new way to study fracture mechanics. Our future work will include simulations of more complicated conditions such as grain boundary problems in three-dimensional simulation.

DISCUSSION

In this paper, we reported a novel approach using machine learning to efficiently investigate dynamic crack propagation in brittle materials. In terms of data representation, the proposed processing method to analyze the MD simulation results brings up several advantages by imbedding discrete and massive atomic information into image-based data structures as shown in Figure 5. First, one can automatically construct a dataset with labels in matrix form from MD simulation results, which reduces the manual efforts needed in common supervised learning approaches. Second, the information of temporal and spatial behavior of cracking can be intuitively imbedded into the dataset for a machine-learning model. In future work, it may be possible to include stress/strain fields (see also Figure 6) in image representation as shown in Figure 7 with higher dimensions (e.g., by using chromatic colormaps). Lastly, the new approach has the potential to integrate well with other simulation methods, such as particle methods, phase field modeling, CZM, or extended finite methods (XFEM), if they possess enough geometric information. This offers several avenues for future work that integrate multiparadigm modeling into the neural network framework proposed here. It can even couple experimental and simulation-based data into the training set, offering a powerful new way to develop predictive models from a rich and diverse set of raw data.

The aim of this study was not only to bypass the complex, intensively computational simulation by adopting a scalable machine-learning model but also to predict a dynamic fracture path for different crystalline structure and boundary conditions. In fact, we have shown that this model can be used to predict crack patterns when subjected to different loading conditions, henceforth offering a general framework for varied fracture scenarios (the training history is shown in Figure 8). Our results also show a good agreement with the trend of crack length in the distribution of crystalline orientations, setting the stage for more complex systems that can be explored. In future studies, the performance of the model can be improved by adding more data from MD simulation results with complicated geometric conditions, which not only follows the general methods used in machine leaning but also confirms that our approach creates a generalizable, feasible way to represent data from MD modeling for AI applications.

It is worth noting that the predictive method only takes the geometry and position of the initial crack to make a prediction, which offers a highly efficient process of modeling this complex physical phenomenon, leading to a new material design approach at the nanoscale. Our machine-learning algorithm for fracture mechanics may provide new avenues to design engineering materials, for instance, high-performance composites, and how these materials respond to various scenarios of crack propagation. Some of the results of the bicrystal cases show some level of deviation between the MD results and the machine-learning mode. The reason is likely that the model did not learn the behavior from MD simulations of bicrystals. Rather, the case was chosen to explore whether or not the model, trained only on single crystals with different orientations, can make adequate predictions for variations in angles or bicrystal interfaces. The results are very promising, showing the predictive power of the method to extrapolate beyond the cases included in the training set. Future work could build on this, for instance by implementing an autonomous retraining

(or transfer learning) approach that expands the training set, if needed, within a multiscale modeling setup.

Based on the findings of this study, we find that the AI-based approach to predict fraction patterns and possible toughness opens the door to generative methods that enable us to perform reverse engineering of mechanical properties. In future work, the method reported here can be further extended by working with adversarial training and could also be combined with WaveNet[44] to generate crack-insensitive materials based on prior probabilities evaluated from the training dataset. Composite materials can be designed by using the algorithm to design microstructures to realize certain crack patterns. This paper has focused on simple Lennard-Jones materials but could be easily generated for other materials, force fields, and material property predictions. Future work could be focused on developing deep neural networks that include other loading conditions, perhaps more complex force fields including quantum-level descriptions of matter, or other multiscale aspects such as coarse graining.

EXPERIMENTAL PROCEDURES

Resource Availability

Lead Contact

Please contact Prof. Markus Buehler via mbuehler@MIT.EDU.

Materials Availability

No other materials are included in this work.

Data and Code Availability

All data and source code are available upon request.

Molecular Dynamics Simulations

As can be seen in Figure 5, we choose a single-layer space of triangular lattice with a width of 80 and a length of 100 unit-lattice. An initial crack of around 10 unit-distances is chosen at the middle-left edge. As the force field of our MD models, we choose a Lennard-Jones (12-6) potential as Equation 3 with cutoff r_c at 1.5 unit-distances and ε of 30 unit energy, which ensures that the crack patterns present sufficiently realistic physical meanings.[45] The timestep is 0.01 unit-time, and we apply 0.0005% of strain in each timestep. The total simulation time is 200 unit-times to reach overall fracture of the specimen. As can be seen in Figure 6A, the elastic limits of our MD model are around 2%–4% of strain. Also, the crack lengths in different orientation angles show significant variance of around 2%–4% of strain as shown in Figure 6B. To reveal the real physics in the initial crack propagation, we pick timestep 6,750, which is 67.5 unit-time, of our MD results to meet 3.375% of strain.

$$V = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \quad r<r_c. \qquad \text{(Equation 3)}$$

Data Processing

The machine-learning method proposed here relies on a rigorous way to represent the features of fracture and distinct geometries in a consistent manner. Here, we focus on the relationship between specific states of strain and the geometric conditions applied. We hence need a specialized container in a high-dimensional format to store the information. To solve this problem, we developed a data-processing method using image-based matrices to represent key geometric information from MD simulation results.

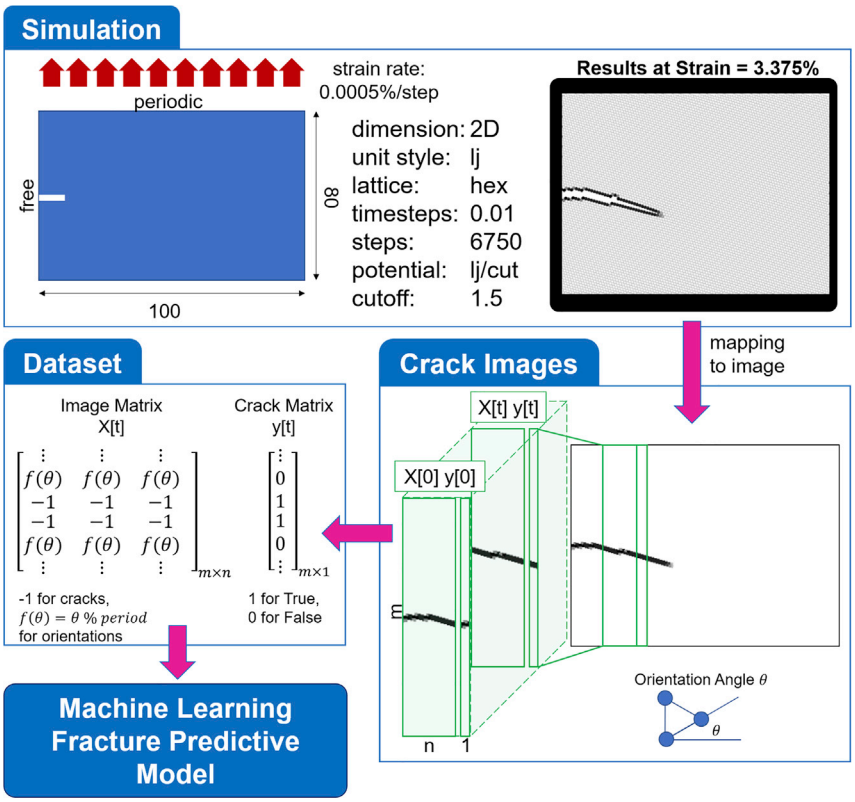

Figure 5. Workflow Used to Construct Our Predictive Machine-Learning Model for Fracture

We start with a large set of 2D fracture simulations. Through a novel image-based data-processing method, the results of fracture simulations are transformed into images that present the definite positions of cracks. The corresponding orientation angles are reserved to represent physical meanings. Subsequently, all images are split into image matrix as input X and the crack matrix as output y for our machine-learning predictive model. With the representation of geometry in image matrix, our predictive model is sensitive to various crystalline orientations.

As shown in Figure 7, all simulation results are mapped into images with a length of 160 pixels and a width of 120 pixels. We found that the resolution is sufficient to make adequate predictions of the crack paths even under varied boundary conditions. The imaging is done using OVITO, which includes a series of visualization modules to indicate the position of crack segments from the atomistic data. First, we draw all atoms in a square shape and draw them sufficiently large to fill the empty space in the image canvas. Subsequently, atoms with fewer bonds to neighbors are colored darker than others using a black-and-white colormap. All atoms and their positions are frozen at the first step. After these visualization steps, the information of discrete atoms is mapped into a continuous image, which only has the simplified information of a crack or no-crack left, which aids ignoring noise generated from the shape of atoms and the movement of atoms in a snapshot, hence focusing on the essential information of the crack segment positions in space, over time. Hence, the machine-learning model can directly recognize the crack patterns.

Furthermore, to capture the causal dependencies by which geometric conditions would affect how a crack propagates, we split all of them into couples of matrices as input X and the output y, which can be considered as elements and labels. For the input X, the geometric matrix, we replace the values of non-crack (white) area with the corresponding orientation angles and replace the values of crack (black) area with value of −1. By doing

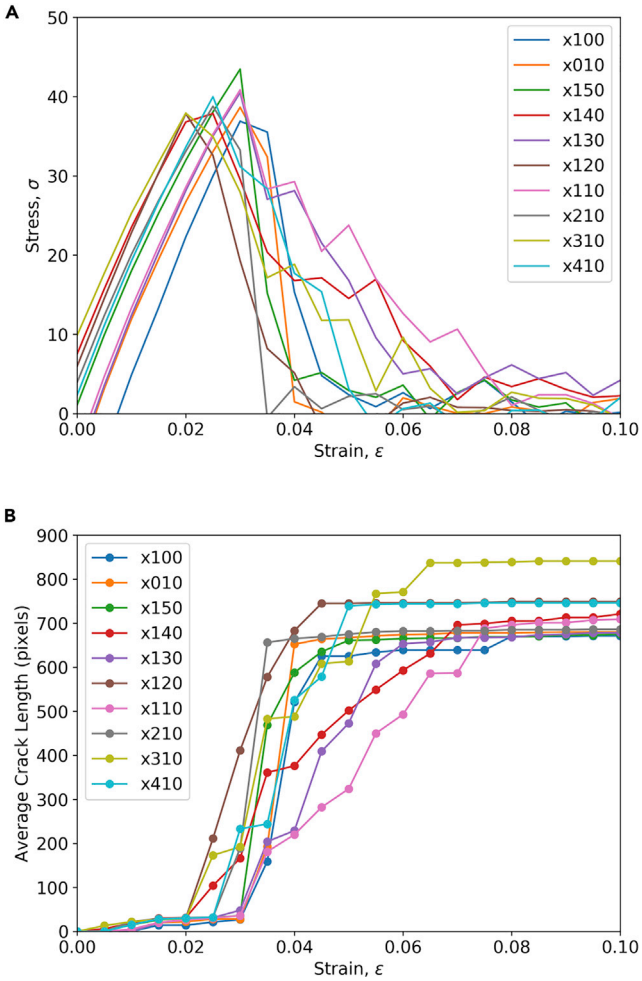

Figure 6. Physical Behaviors as Observed in Our MD Simulations

(A) Stress-strain curve predicted from MD simulations under different orientation angles.

(B) Average crack length growth versus strain for different orientation angles.

so, we should be able to reserve the geometric conditions as much as possible after we map simulation results to images because the orientation angles should be only ranging from 0 to 2π. Then, we transform the output y, the crack matrix, into one-hot encoding labels for positions of crack, 0 for non-crack positions and 1 for crack positions.

After data preprocessing in our method, the dataset for a predictive machine-learning model consists of a total number of 14,300 pairs of geometric and crack matrices. Each pair is a window to screen and capture information from a crack image, as depicted in Figure 5. Once processed in this way, the dataset is ready for machine learning to reveal the physical meanings in MD simulation results.

Machine-Learning Model

The basic concept is to learn the spatiotemporal relations from a series of physics-based MD simulations, including orientations, time, strain, and crack growth. In the previous studies, ConvLSTM-based models show the capability to extract patterns in such spatiotemporal data. As a result, we adopt a ConvLSTM model to address the implicit spatiotemporal relations in MD simulation results. All implementation is in Python with the Keras package under Tensorflow (tensorflow.keras) with

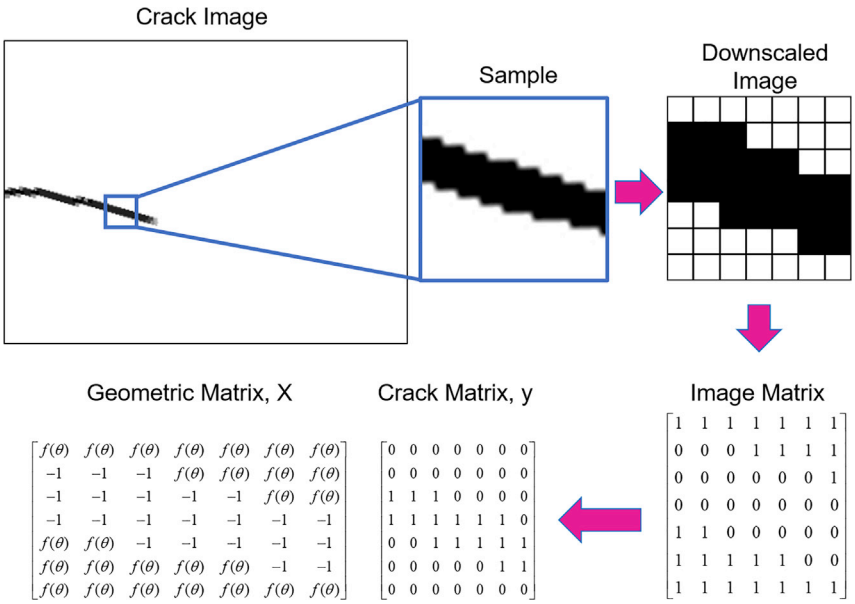

Figure 7. Details of Data Preprocessing for the Machine-Learning Model

The MD simulation result will be mapped into image by OVITO and then downscaled to image matrix with lower dimensions. The white part of the image is the non-crack region and the black part indicates where the crack occurs. To preserve the effect of geometric conditions, we transform the image matrix into geometric matrix, X, and crack matrix, y, for the machine learning.

one Nvidia 2080 Ti.[46] For use in the predictive model at a specific strain, the training set mapped from MD simulation results is shown in Figure 8A, where the strain is set to 3.375%. The structure of our predictive model is shown in Figure 8B, which includes two 1D convolutional (Conv1D) layers, one LSTM unit, and one dense layer as the output layer. Here, we apply Conv1D layers to extract the geometric information of the crack and non-crack area column by column from crack images and then apply LSTM to recognize the implicit connection between them.

In the first two Conv1D layers, the numbers of filters are both set to 64 and the kernel sizes are both set to a half of the width of images, which would be 60 and 61 in this study. These two Conv1D layers reduce the dimensions of the input geometric matrix from 12.0 × 16 to 64 as a latent space for physics[47] to address our image-based fracture mechanics. We then adopt an LSTM unit with 512 nodes to learn the sequential relations along with the crack propagation. At the end, we use a dense layer as the output layer with 120 nodes, same as the width of a crack image, to up-sample our prediction back to the real space to show where the crack could happen. Moreover, we adopt *binary_crossentropy* as the loss function and *sigmoid* as the activation of the output layer to describe the subtle behaviors of crack propagation. With *binary_crossentropy*, we can interpret the probability of crack in each pixel from 0 to 1 as the probability of crack on different positions.[48–50] Through this approach, the crack prediction problem become a multiclassification problem.

For the training part, the training process is done with one Nvidia GeForce RTX2080Ti, and the training history, depicted in Figure 8C, shows that complicated and implicit relations between fracture patterns and geometric conditions can be learned adequately by the machine-learning model. In terms of detailed settings, we adopt an Adam optimizer with a learning rate of 0.0001 with decay of 0.001. Other settings of optimizer are the default values. We set the batch size of training

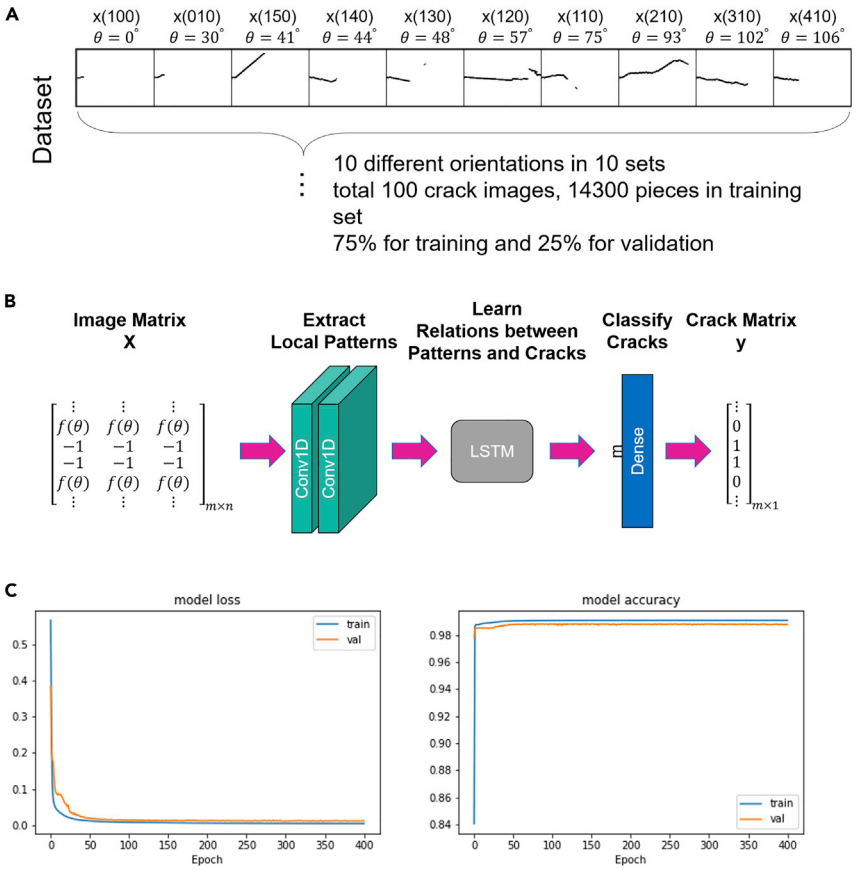

Figure 8. Details of the Machine-Learning Predictive Model, Exemplifying How We Move from the Training Set to the Dataset to Training

(A) Dataset consists of a total of 100 crack images prepared directly from MD simulation results of fracture propagation.

(B) Structure of our fracture-predictive model.

(C) Training history of our predictive model.

to 64 to make sure that the details of relation between cracks and geometry can be learned in each training batch. It is worth noting that in our method, the use of memory and computation cost mainly depends on the image size, not the real model size in MD (in other words, the number of atoms within it).

Method of Making Predictions of Fracture Pattern

For the generation of the prediction of fracture pattern, we take an iterative process to obtain the entire crack patterns. This is because each output of our predictive model has only one column of pixels. In this work, the outputs range from the first column after initial crack to the end of the image, which represent a range from the 17th to the 160th column (this can be adjusted if a user wants to work with differently sized images). In each prediction of the next crack advance, we transform the output (the crack matrix) to the geometric matrix and update the new geometric matrix for the next input, realizing an iterative approach. More precisely, the geometric matrix, input X, is a processing queue to take the latest crack in its tail, and pop out the oldest geometric condition column by column, iteratively. In this way, the input we need for the prediction would be only the first 16 columns of the crack image, which contains initial crack and the geometry. In other words, we can input geometric conditions into our predictive model and then obtain the possible crack patterns with a specific strain, according to the training set

used (e.g., multiple strain levels can be realized by training the model against such variations of strain and using multiple sets of parameters).

SUPPLEMENTAL INFORMATION

Supplemental Information can be found online at https://doi.org/10.1016/j.matt.2020.04.019.

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AUTHOR CONTRIBUTIONS

M.J.B. and C.-H.Y. conceived the idea. Y.-C.H. and C.-H.Y. carried out the MD simulations. Y.-C.H. and C.-H.Y. curated the training and testing data. Y.-C.H. developed the machine-learning model. C.-H.Y. assisted with the development of the machine-learning model. Y.-C.H. and C.-H.Y. developed the machine-learning predictor. M.J.B. supervised the project. Y.-C.H. and C.-H.Y. wrote the manuscript with M.J.B.

DECLARATION OF INTERESTS

The authors declare no competing interests.

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