USING DEEP LEARNING TO PREDICT MICROSTRUCTURALLY SMALL FATIGUE CRACK GROWTH PARAMETERS IN POLYCRYSTALLINE MATERIALS

Vignesh Babu Rao[1]*, Brian Phung[1], Bjorn Johnsson[1], and Ashley Spear[1]

[1]*University of Utah, Salt Lake City, UT, USA*
** Presenting Author email: vignesh.baburao@utah.edu*

Abstract

The ability to rapidly predict the growth behavior of microstructurally small cracks (MSCs) has the potential to significantly advance fracture-based designs and structural prognosis. The difficulties associated with characterizing or predicting MSC growth using experimental and numerical techniques preclude the applicability of such techniques in industrial design approaches, despite their potential benefits. Here, we propose a framework to accelerate high-fidelity MSC growth predictions using deep-learning algorithms, viz., convolutional neural networks (CNNs). The primary research aim is to train CNNs to predict the rules governing MSC growth and to subsequently apply the trained CNNs to make rapid forward predictions of local crack extension given microstructural neighborhood information along a crack front. The training data are acquired from a large number of "virtual" MSC growth observations enabled by high-fidelity finite-element-based simulations. The MSC-growth-simulation framework, data-extraction strategies, and application of deep-learning algorithms for data-driven model development will be presented, and the resulting advantages will be demonstrated.

1. Introduction

Microstructurally small cracks (MSCs) are cracks whose sizes are on the order of the size of predominant microstructural features. Because MSCs are heavily influenced by local microstructural features, traditional, continuum-scale fracture-mechanics theories that assume homogeneous, isotropic material conditions fail to make reasonable predictions for MSC growth behavior. Early works suggest that fatigue cracks can spend 50-70% of their lifetime in the MSC regime. This means that understanding MSCs and being able to predict their growth could enhance materials design, improve residual life estimation, and allow for reduced safety factors. Motivated by this fact, there have been many studies that have aimed to understand MSC behavior.

Though a number of research studies have investigated the mechanisms governing MSC growth, their results have not been utilized in the industrial design processes. This is primarily due to the challenge associated with the collection of MSC growth data via either experiments or simulations at the microstructural length scale. Experimental techniques, such as electron backscatter diffraction, X-ray tomography, and high-energy X-ray diffraction microscopy, have proven to be extremely valuable in uncovering MSC growth rules. While they provide invaluable information, they are expensive, time-consuming, and require sophisticated equipment. Mesoscale microstructure-sensitive modeling poses a viable alternative solution to predict MSC growth. Crystal-plasticity-based finite-element (CPFE) models, can be used to evaluate the micromechanical state around a crack tip and thereby aid in predicting crack growth parameters. Though they provide satisfactory results, CPFE simulations are computationally expensive and require massive computing resources for realistic, three-dimensional polycrystals. A fast and reliable way of predicting the MSC growth parameters essential for industrial design practices is currently impossible using state-of-the-art experimental and numerical techniques.

In this work, we propose a framework to accelerate MSC growth predictions using deep learning algorithms, viz., convolutional neural networks (CNNs). Using a unique data sampling strategy (as illustrated in Fig.1b), the training data are acquired from high-fidelity, CPFE-based simulations that use a crystal plasticity constitutive model and a voxel-based remeshing framework for simulating crack growth (as shown in Fig.1a) in a large number of polycrystalline microstructures. The collected data are used to train a CNN model (Fig.1d) to predict MSC growth parameters, including the local crack extension, Δa.

2. Results

Results from training and testing CNNs to predict Δa are summarized as follows:

a. A feature sensitivity analysis was performed to assess the importance of individual features in predicting MSC growth characteristics by training CNNs with input features one at a time. Features such as quaternions, directional elastic modulus, and micromechanical Taylor factor were found to be more influential than geometric features such as crack size and distance to the crack front from free surfaces.
b. A study to determine the minimum amount of data required for training CNNs was conducted, where multiple CNNs were trained with progressively increasing amounts of training data. Result showed that with increasing amount of training data, the performance variability among cross-validation runs tended to decrease while the average performance among cross-validation runs tended to increase. The results suggested that beyond 30 microstructural instantiations (approximately 6000 total data points across 60 discretized crack fronts), the model performance tended to saturate.
c. The change in crack tip displacement (ΔCTD), which is a measure of the crack driving force, exhibits distinct variations along the crack front because of the presence of microstructure. The CNN predictions of Δa, which is a linear function of ΔCTD, are shown to capture those variations (Fig.1c) and thereby suggest that CNNs, indeed, learn the microstructure-sensitive behavior of MSCs.
d. Once trained, the CNNs take <30 seconds (on GTX1070 GPU) to predict Δa along the crack front in an entirely new microstructural instantiation; whereas, evaluating Δa values by running high-fidelity simulation takes about 2304 CPU hours on average. The proposed approach enables rapid prediction of Δa, which, in conjunction with other MSC growth parameter predictions, could potentially benefit materials design and optimization.

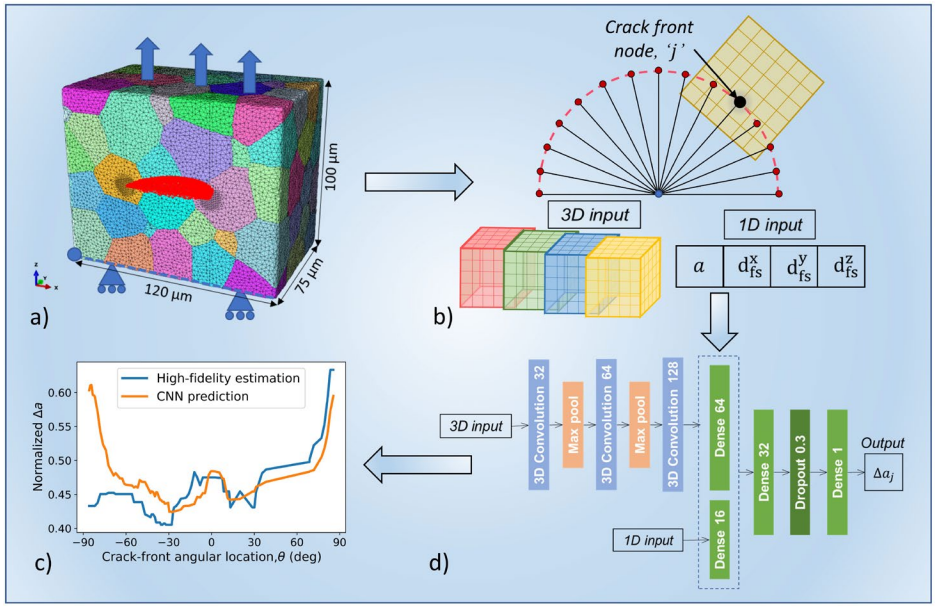

Fig.1 – a) High-fidelity simulation domain with an initial half-penny crack. b) Sampling grids along crack front are used for data extraction. c) Comparison of CNN predicted Δa with the simulation result along the crack front d) CNN architecture used to train and make forward predictions of Δa_j.

3. Conclusions

Sampling data from a large number of CPFE-based MSC growth simulations resulted in a dataset containing many "virtual" Δa observations. Results suggested that CNNs can learn the microstructure-sensitive behavior of MSCs and make reasonable predictions for Δa. The trained CNN models predicted Δa several orders of magnitude faster than the high-fidelity simulations.

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