AFRL-AFOSR-VA-TR-2019-0198

3-D Multi-Scale Modeling Combined with Machine Learning for a Novel Structural-Prognosis Framework

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08/16/2018
Final Report

DISTRIBUTION A: Distribution approved for public release.

Air Force Research Laboratory
AF Office Of Scientific Research (AFOSR)/ RTA1
Arlington, Virginia 22203
Air Force Materiel Command

REPORT DOCUMENTATION PAGE	*Form Approved OMB No. 0704-0188*

1. REPORT DATE *(DD-MM-YYYY)*	**2. REPORT TYPE**	**3. DATES COVERED** *(From - To)*
23-07-2019	Final Performance	15 Apr 2015 to 14 Apr 2018

4. TITLE AND SUBTITLE
3-D Multi-Scale Modeling Combined with Machine Learning for a Novel Structural-Prognosis Framework

5a. CONTRACT NUMBER

5b. GRANT NUMBER
FA9550-15-1-0172

5c. PROGRAM ELEMENT NUMBER
61102F

6. AUTHOR(S)
Ashley Spear

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
UNIVERSITY OF UTAH SALT LAKE CITY
201 PRESIDENTS CIR RM 408
SALT LAKE CITY, UT 84112-9023 US

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AF Office of Scientific Research
875 N. Randolph St. Room 3112
Arlington, VA 22203

10. SPONSOR/MONITOR'S ACRONYM(S)
AFRL/AFOSR RTA1

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
AFRL-AFOSR-VA-TR-2019-0198

12. DISTRIBUTION/AVAILABILITY STATEMENT
A DISTRIBUTION UNLIMITED: PB Public Release

13. SUPPLEMENTARY NOTES

14. ABSTRACT
The goal of the research is to enhance structural-prognosis capabilities for the USAF by discovering a quantitative model capable of predicting the morphological evolution of three-dimensional (3-D) microstructurally small fatigue cracks (MSFCs) based on local, microstructure-sensitive fields. Three of the most significant hindrances to predicting the MSFC life for an arbitrary material microstructure under arbitrary far-field loading include: (1) uncertainty in the 'rules' (i.e. quantitative, parametric representations of the crack-driving mechanisms) that are used to evolve a 3-D crack at the scale of the microstructure; (2) missing or incomplete information in the cracks' surroundings and applied boundary conditions; and (3) inadequate representation of cracks as evolving discontinuities and their corresponding fluctuations. During the three-year period of this AFOSR Young Investigator Program (YIP) award, the PI and her graduate students have made significant research advancements toward improving structural-prognosis tools for the USAF by addressing each of these challenges.

15. SUBJECT TERMS
fatigue, microstructure, machine learning, probabilistic

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**			TILEY, JAIMIE
Unclassified	Unclassified	Unclassified	UU		

					19b. TELEPHONE NUMBER *(Include area code)* 703-588-8316

Grant Title:	3-D MULTI-SCALE MODELING COMBINED WITH MACHINE LEARNING FOR A NOVEL STRUCTURAL-PROGNOSIS FRAMEWORK
Type of Report:	FINAL REPORT
PI:	ASHLEY SPEAR, University of Utah, *ashley.spear@utah.edu*
Program Officer:	DR. JAIMIE TILEY, Multi-scale Structural Mechanics and Prognosis
Report Period:	15 APRIL 2015 – 14 APRIL 2018
Grant Number:	FA9550-15-1-0172

1. Project Description Overview

The goal of the research is to enhance structural-prognosis capabilities for the USAF by discovering a quantitative model capable of predicting the morphological evolution of three-dimensional (3-D) microstructurally small fatigue cracks (MSFCs) based on local, microstructure-sensitive fields. The proposed technical approach involves three high-level tasks:

Task 1. Numerically reproduce observed 3-D MSFC behavior.

Task 2. Use machine learning to discover the MSFC-evolution "rules" as a function of fields computed from the reproduced behavior.

Task 3. Demonstrate use of the machine-learned model to predict 3-D MSFC behavior.

2. Significant Research Accomplishments

Three of the most significant hindrances to predicting the MSFC life for an arbitrary material microstructure under arbitrary far-field loading include: (1) uncertainty in the "rules" (i.e. quantitative, parametric representations of the crack-driving mechanisms) that are used to evolve a 3-D crack at the scale of the microstructure; (2) missing or incomplete information in the cracks' surroundings and applied boundary conditions; and (3) inadequate representation of cracks as evolving discontinuities and their corresponding fluctuations. During the three-year period of this AFOSR Young Investigator Program (YIP) award, the PI and her graduate students have made significant research advancements toward improving structural-prognosis tools for the USAF by addressing each of these challenges. Specifically, the team has focused on reducing uncertainty in fatigue-life predictions within the microstructurally small regime by improving understanding of the rules used to govern 3-D crack evolution at the microstructural length scale (Tasks 1 and 2) and by developing a robust computational framework that is capable of combining these rules with a high-fidelity representation of evolving cracks (Task 3). Progress made in each of these areas is described in the following sub-sections.

As a result of the research associated with this YIP award, four journal articles have so far been published or submitted (in review), one more journal article is currently in preparation, two graduate students have spent summers at AFRL, one M.S. student has completed his degree, two Ph.D. students are within 1-2 years of graduation, and a framework has been developed to support ongoing research efforts in the area of multi-scale structural mechanics and prognosis.

2. 1 Improving Rules for Predicting MSFC Propagation

Through Tasks 1 and 2, the team has made progress toward advancing the understanding of rules that govern 3-D crack evolution in a real (non-idealized) aerospace material. In Year 1, experimental observations from prior work were reconstructed and recast as high-fidelity models to numerically reproduce the MSFC behavior observed in experiment. In prior work by the PI, the fatigue-failure surface and 3-D microstructure (including grain morphologies and crystal orientations) from a fatigue specimen of an Al-Mg-Si alloy were measured using X-ray computed tomography and high-energy X-ray diffraction microscopy at the Advanced Photon Source Sector 1-ID beamline. As part of this YIP award, the experimental data were reconstructed and represented with a conformal finite-element mesh containing the incremental discontinuity of the crack surface. A concurrent multiscale model was then generated to ensure that the correct boundary conditions were transferred to the polycrystalline domain during simulated loading. Figure 1 shows the concurrent multiscale mesh based on the experimental measurements. Figure 2 shows the computed micromechanical fields for successive crack-growth increments. The work was published in 2016 [1].

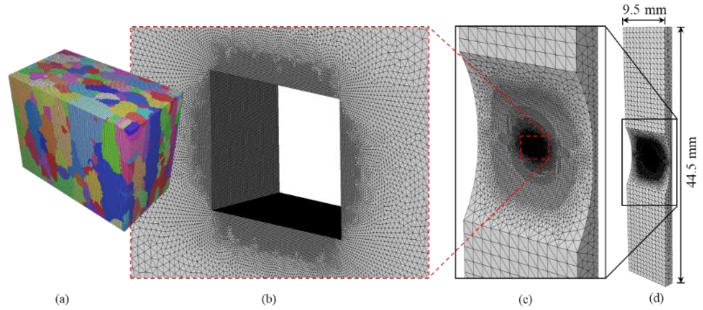

Figure 1 Components of the concurrent-multiscale mesh for an Al-Mg-Si alloy fatigue specimen. (a) A conformal grain-scale mesh generated using a method developed by the PI, (b) magnified view of macroscale mesh generated in Abaqus®, (c-d) concurrent-multiscale mesh. From Ref. [1]

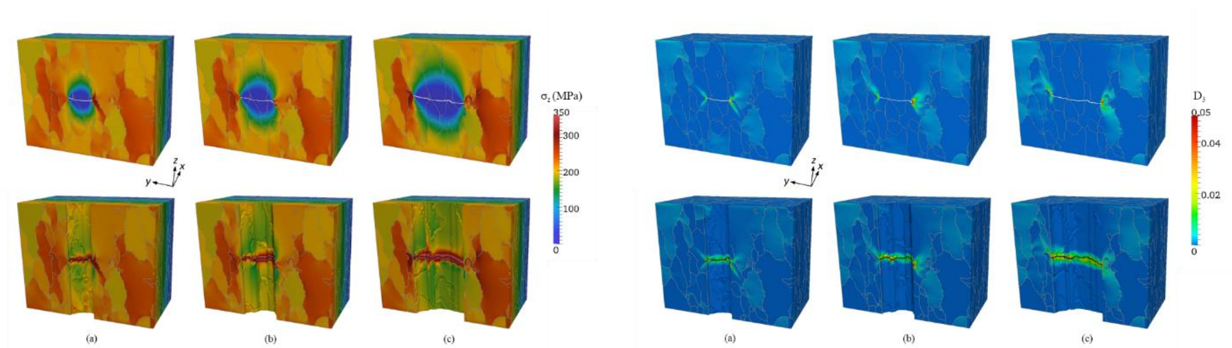

Figure 2 Micromechanical fields from simulations of monotonic loading for three crack-shape increments that were measured experimentally at: (a) 180,000 cycles, (b) 190,000 cycles and (c) 200,000 cycles. Top row depicts full volume with crack trace shown in white on free surface. Bottom row shows interior view with fields just ahead of the embedded crack front (crack-front points are shown in black). Stress component in the z direction is shown on the left, and a slip-based damage metric is shown on the right. From Ref. [1]

Due to the large amount of data generated from both the high-energy X-ray measurements and the high-fidelity numerical simulations, a data-driven approach was subsequently employed to elucidate the micromechanical features that most strongly correlate with the measured crack path. The specific objective of the study was to determine what, if any, micromechanical field variables in the cyclically loaded, uncracked polycrystal correlate with the eventual path of the experimentally observed crack. The concurrent multi-scale mesh shown above in Figure 1 was analyzed using a parallelized finite-element code. In the domain of the polycrystal, a crystal-plasticity model was employed, and cyclic loading was simulated to replicate experimental conditions. Figure 3 shows the convergence trend of the micromechanical fields during simulated cyclic loading. At the final loading cycle (once the fields had saturated), the results from the finite-element analysis were subsampled onto a structured, 3-D grid of data points.

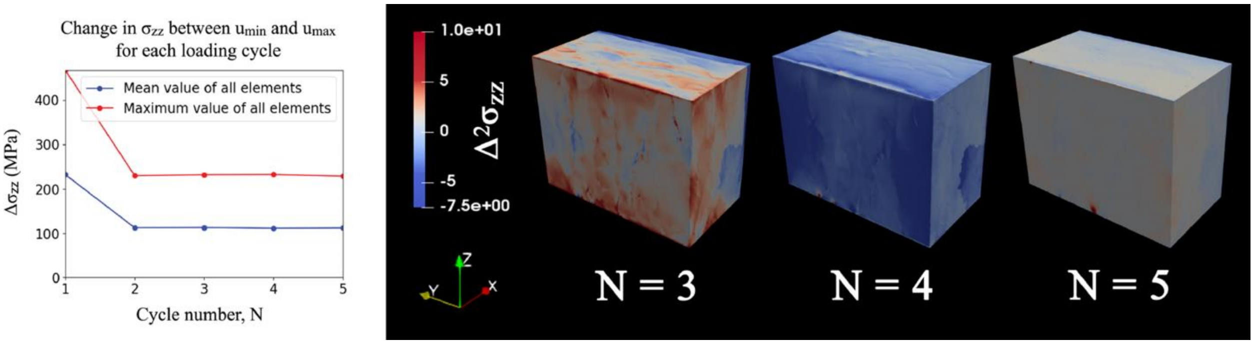

Figure 3 Convergence of stress in the loading direction during simulated cyclic loading. From Ref. [2]

In the correlation analysis, 88 micromechanical variables were considered: 22 variables that were computed throughout the simulation, including stress and strain tensor components, slip-based damage metrics, micromechanical Taylor factor, and various derivatives of the stress and strain tensors; the cyclic change in each of the 22 variables between minimum and maximum loading; and the spatial gradients of all 44 aforementioned variables. Then, for all grid points within a distance, *L*, to the crack surface (see Figure 4), a correlation analysis was performed between each of the 88 variables and the distance to the known crack surface. In total, 14.3M grid points were analyzed, and each point had 88 attributes associated with it. The analysis was paralyzed, and the statistical package R was used to compute the correlation coefficients. Results of the Pearson correlation coefficients for all 88 variables are shown in Figure 5. To determine whether the values in Figure 5 are meaningful, the correlation analysis was repeated, but for alternative, hypothetical crack paths. The results from that correlation analysis are shown in Figure 6 for comparison.

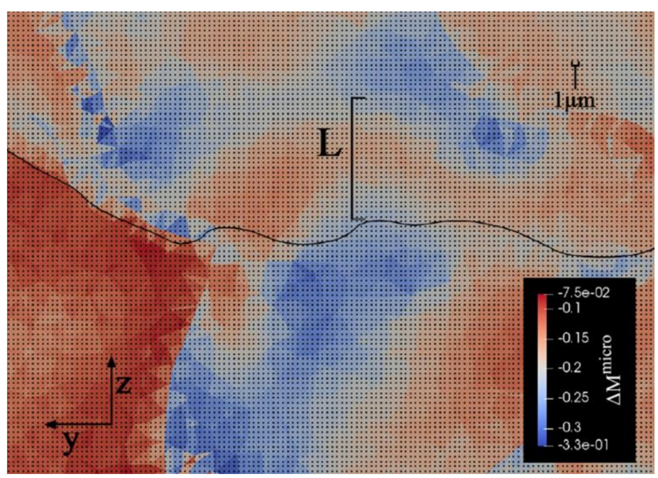

Figure 4 Cyclic micromechanical Taylor factor computed for the uncracked polycrystal, shown at a particular slice through the volume. Superimposed is the trace of the actual crack surface from x-ray CT imaging. Also superimposed is the grid used for correlation analysis. The neighborhood of influence is defined by the distance L above and below the crack surface. From Ref. [2]

Two significant findings resulted from this study. The first is that there appears to be some degree of predictive power in the field variables of a cyclically loaded, uncracked microstructure in terms of predicting crack path. The extent of this predictive power is the subject of ongoing investigation. The second and perhaps more important finding is that the spatial gradients of the micromechanical fields tend to exhibit much stronger correlations with crack path than the micromechanical fields, themselves. This suggests that the MSFC-driving mechanism is more closely related to the strength of the field *gradients* than to the strength of the field variables. Based on the results from the data-driven correlation analysis, the variables of interest were downselected from 88 to 22. The smaller number of more highly correlated variables are currently being used to train and assess various machine-learning models (e.g. convolutional neural network and support vector regression) to identify a quantitative and parametric rule that represents the driving mechanisms of MSFC growth. Establishing such rule is challenging and will be the topic of a forthcoming publication by the PI and her team.

The results from the correlation analysis were published recently [2] and received recognition as the *Editor's Choice* for the month of publication. The PI also published a guest editorial on the topic of data-driven approaches, including machine learning, applied to fatigue of materials [3].

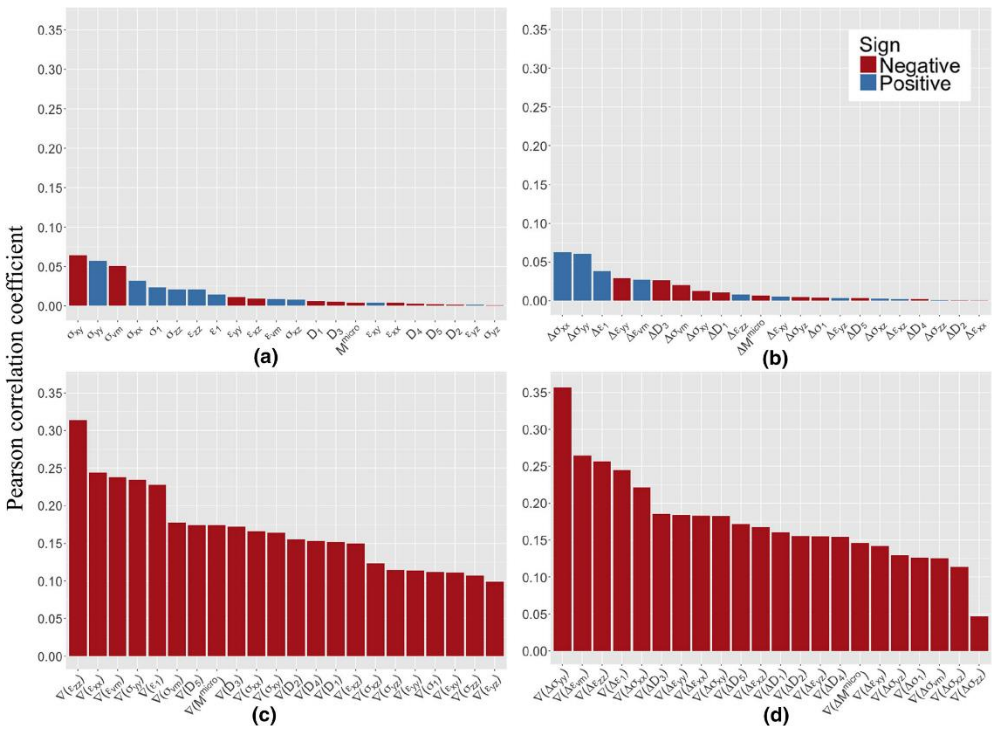

Figure 5 Correlation coefficients computed between the following metrics and distance to crack surface: (a) field variables; (b) cyclic change in the field variables; (c) spatial gradient of the field variables from (a); (d) spatial gradient of the cyclic field variables from (b). From Ref. [2]

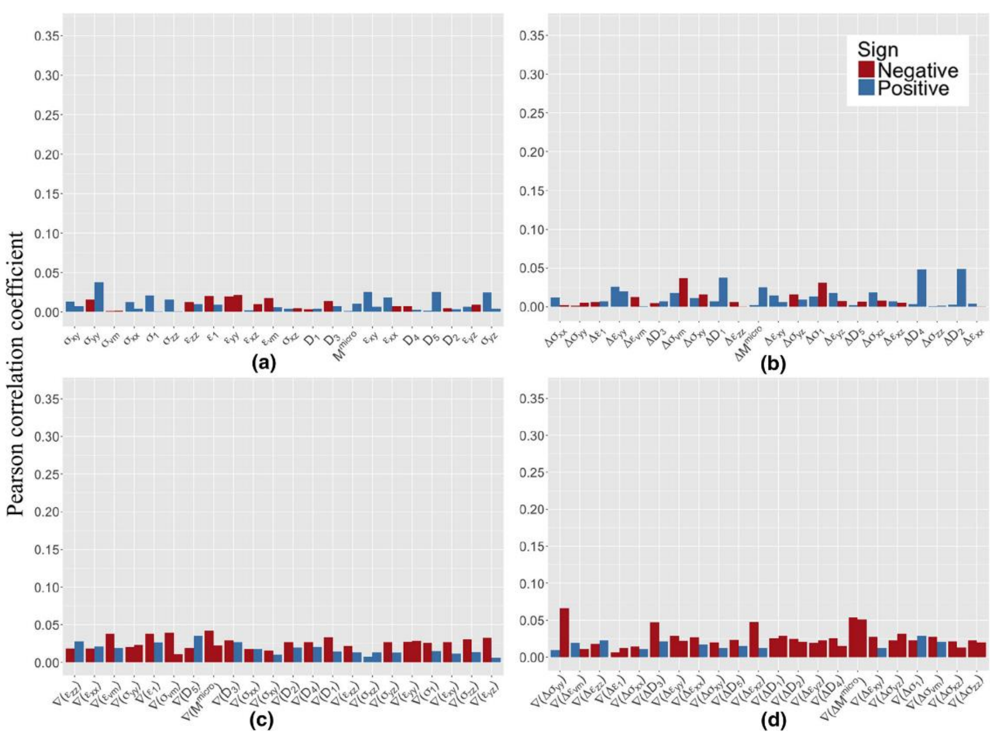

Figure 6 Correlation coefficients computed between the following metrics and distance to alternative, hypothetical surfaces: (a) field variables; (b) cyclic change in the field variables; (c) spatial gradient of the field variables from (a); (d) spatial gradient of the cyclic field variables from (b). From Ref. [2]

2.2 Development of a Robust and Flexible Framework for Simulating MSFC Propagation

In parallel with the research efforts described above, the team has developed and demonstrated a voxel-based remeshing framework capable of simulating realistic, high-fidelity crack propagation at the microstructural length scale. While numerous adaptive-remeshing schemes exist for the simulation of arbitrarily shaped cracks at the continuum scale, conventional implementations struggle to accommodate complex 3-D crack shapes and interactions with internal material boundaries in heterogeneous domains. The approach implemented recently by the team addresses this issue by relying on a voxel-based description of the heterogeneous domain, as opposed to a surface-based geometrical description. The result is a robust and flexible framework that allows for the simulation of arbitrary, 3-D crack propagation in material microstructures. The discontinuity is explicitly represented and is allowed to propagate through, along, or very near to grain boundaries, as dictated by the crack-driving mechanism. A high-level overview of the workflow is shown in Figure 7. As shown in the figure, the framework is modular, such that different plasticity models, finite-element solvers, and crack-growth criteria can be implemented. Thus, the framework serves as a unique and powerful tool to investigate both new and existing crack-growth rules.

In the framework, computed field variables are monitored ahead of and behind discrete locations along the 3-D crack front, as depicted in Figure 8. The field variables are then used to evaluate user-specified growth criteria. Based on the evaluation, a new set of crack-front points is generated, and the voxel-based mesh is regenerated to accommodate the new traction-free

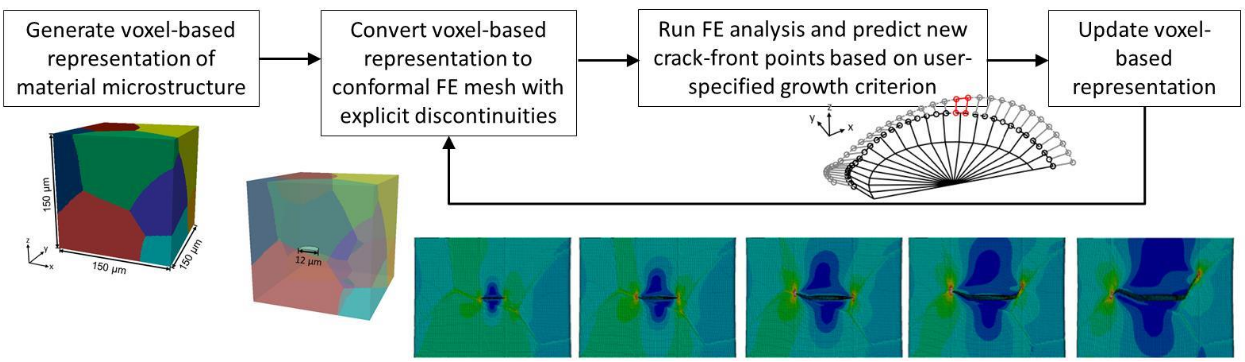

Figure 7 Algorithm of voxel-based remeshing framework to simulate MSFC propagation.

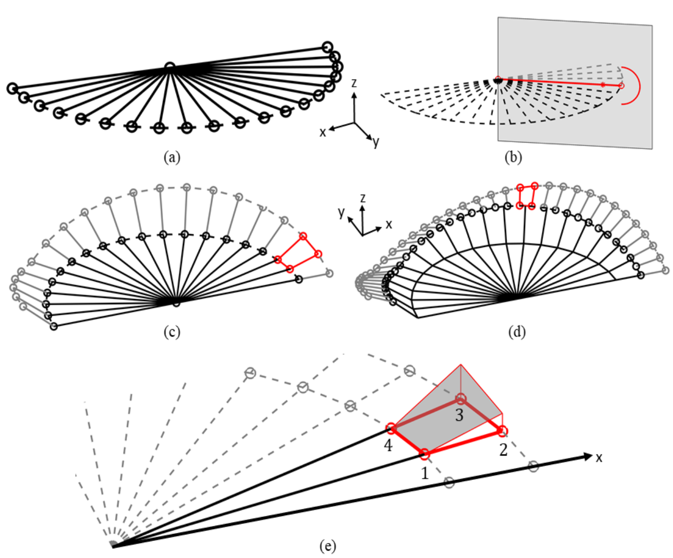

Figure 8 (a) A ray representation of a simple penny-shaped crack surface. Crack-front points are depicted, and the crack front is interpolated from the crack-front nodes. (b) Probe points behind (e.g. indicated by an asterisk) and ahead of (e.g. indicated by the red semi-circle) a given crack-front node are defined with a plane that contains the crack origin and crack-front node. The probe points can be used to evaluate user-defined growth criteria. (c) The ray representation of a simple penny-shaped crack surface with predicted crack-front points. A single section is highlighted red to illustrate the formation of quadrilateral finite elements along the new crack surface. (d) An illustration showing that crack-front points following remeshing do not necessarily correspond to previous points, which allows the crack resolution to be approximately maintained during crack growth. (e) An illustration of the quadrilateral formation procedure and variables aiding in interpolating crack elevation points. From Ref. [4]

surface area between the old and new crack-front points. In this approach, arbitrary (i.e. non-self-similar) crack shapes can be predicted.

The capabilities of the framework were demonstrated through several proof-of-concept simulations. The simulations show the capability to simulate both inter- and transgranular crack growth, coalescence of multiple cracks, crack deflection at grain boundaries, and realistic crack-surface tortuosity. In one of the proof-of-concept simulations, two penny-shaped surface cracks were inserted into a 3-D polycrystal. A Hill anisotropic plasticity model was applied, and each material domain had a different local basis and set of material parameters to mimic the effect of grain orientations. A user-defined crack-growth criterion was also applied. Specifically, crack growth occurred when a critical value of crack-tip displacement was reached, and the local increment of crack growth at a given point on the crack front was scaled based on the crack-tip displacement at that location. The kink angle at each point on the crack front was determined based on the Maximum Tangential (Tensile) Stress Criterion, which asserts that the crack will seek a local path of pure Mode I loading. Applying these criteria for crack-growth increment and kink angle, crack propagation was then simulated using the voxel-based remeshing framework.

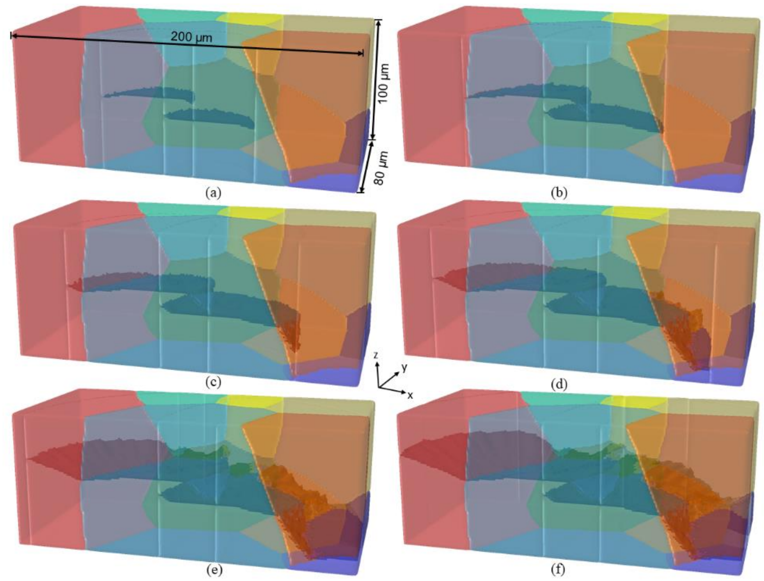

Figure 9 Six of 18 crack-growth increments for the proof-of-concept simulation: a) inc. 3, b) inc. 6, c) inc. 9, d) inc. 11, e) inc.15, f) inc. 18. From Ref. [4]

The results from the simulation are shown in Figure 9. As shown in the figure, the overlapping portions of the cracks initially grow toward each other, but soon arrest as the outer portions continue to accelerate. The crack shown on the left deflects at a grain boundary, but continues to grow transgranularly; while the crack shown on the right turns sharply to propagate intergranularly. Figure 10 shows the computed stress fields in 2-D slices through the volume. Figure 11 shows results from a similar proof-of-concept simulation, demonstrating the ability to coalesce crack surfaces should such behavior be predicted by the crack-driving

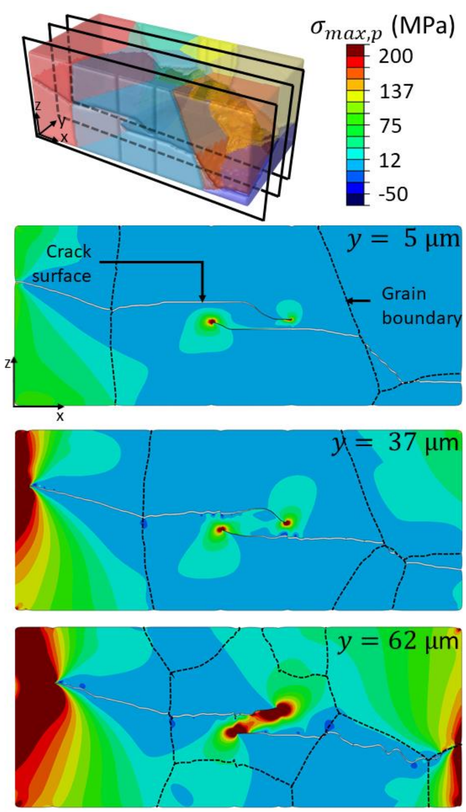

Figure 10 Cross-sectional views in the (x,z) plane depicting the maximum-principal stress fields at the 18th increment of crack growth for two interacting cracks simulated for proof of concept. Slices are made at 5, 37, and 62 µm from the origin. Deformation is scaled by a factor of 1. From Ref. [4]

mechanism. Results from the proof-of-concept simulations show the flexibility, robustness, and modularity of the framework. The work was recently submitted for publication and is currently under review at the time of this report [4].

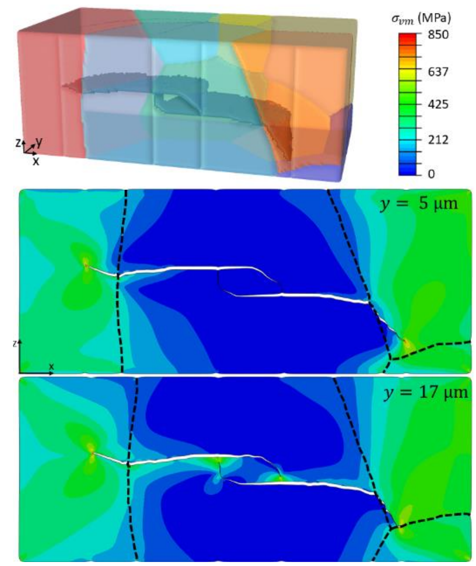

Figure 11 Cross-sectional views in the (x,z) plane depicting the maximum-principal stress fields for the case of coalescing cracks. Slices are made at 5 and 17 µm from the origin. Deformation is scaled by a factor of 1. From Ref. [4]

3. Opportunities for Future USAF Research

With a robust and modular crack-simulation framework in place and an improved understanding of the important micromechanical features that correlate with MSFC propagation, the team is poised to realize the vision of improving structural-prognosis capabilities for real (non-idealized) materials and structures subjected to realistic loading conditions. Despite the significant progress made over the past three years, there remains a need to establish and validate a parametric and quantitative crack-growth rule that generalizes across different aerospace materials. In the proof-of-concept simulations described above, crack-tip displacement was used as a surrogate to represent the driving mechanisms of MSFC propagation. In ongoing work, the team is leveraging the results from the data-driven correlation analysis to establish a mechanism-based, crack-growth rule that can be incorporated into the voxel-based remeshing framework. Once the framework has been validated, future efforts will focus on building a large data set of predictions for different aerospace materials and boundary conditions. The high-fidelity predictions will serve as training data for a probabilistic, surrogate model. The efficiency of such surrogate model will lend itself to a real-time structural-prognosis capability like the Digital Twin.

4. Specific Accomplishments Associated with the Grant

- **Four refereed journal articles** that acknowledge support from this AFOSR grant (three published and one under review at the time of this report), with one additional journal article in preparation
- **Nine invited seminars** by the PI acknowledging support from this AFOSR grant
- **Ten conference presentations** by the PI or her graduate students acknowledging support from this AFOSR grant
- Leveraged support provided by AFRL or its affiliates to develop future workforce:
    - **U.S. Air Force Summer Faculty Fellowship** supported PI and two of her graduate students to spend the summer of 2016 at AFRL in the Structural Sciences Center
    - Support from UTC allowed one graduate student to spend the summers of 2017 and 2018 at AFRL in the Structural Sciences Center
- Developed a **flexible and robust crack simulator** that will be used to sustain future research efforts involving 3-D microstructurally small crack propagation
- Developed a **parallelized data-mining code** to be used for future research efforts involving data-driven science and machine learning

5. Grant-Sponsored Research Dissemination Since Project Start Date (15 April 2015)

5.1 Peer-Reviewed Journal Articles Acknowledging this AFOSR YIP Award

1. Spear, A.D., Hochhalter, J.D., Cerrone, A.R., Li, S.F., Lind, J.F., Suter, R.M., & Ingraffea, A.R. A Method to Generate Conformal Finite-Element Meshes from 3-D Measurements of Microstructurally Small Fatigue-Crack Propagation, special issue contribution to *Fatigue & Fracture of Engineering Materials & Structures*, April 2016. 39(6): 737-751. doi:10.1111/ffe.12449
2. Pierson, K. D., Hochhalter, J. D., & Spear, A. D. (2018). Data-Driven Correlation Analysis Between Observed 3D Fatigue-Crack Path and Computed Fields from High-Fidelity, Crystal-Plasticity, Finite-Element Simulations. *JOM*, 70(7): 1159–1167. https://doi.org/10.1007/s11837-018-2884-2
   ****Selected as Editor's Choice article for the July issue of JOM****
3. Spear, A. D., Kalidindi, S. R., Meredig, B., Kontsos, A., & le Graverend, J. B. (2018). Data-Driven Materials Investigations: The Next Frontier in Understanding and Predicting Fatigue Behavior. *JOM*, 70(7): 1143–1146. https://doi.org/10.1007/s11837-018-2894-0
4. Phung, B.R. & Spear, A.D. (in review). A Voxel-Based Remeshing Framework for the Simulation of Arbitrary Three-Dimensional Crack Growth in Heterogeneous Materials. submitted to *(submitted)*

5.2 Invited Seminars Acknowledging this AFOSR YIP Award

1. **Mechanics in Scientific Discovery** – Presentation by invitation only (June 2017). Florence, Italy. "On the use of machine learning to discover predictors of small-scale crack growth".
2. **Brigham Young University** – Invited seminar at (February 2017). Provo, Utah. "Combining synchrotron imaging with numerical modeling to elucidate microstructure-sensitive phenomena in polycrystalline materials".
3. **Argonne National Laboratory** – Invited speaker at the Advanced Photon Source User Science Series (October 2016). Argonne, Illinois. "3D grain mapping to inform high-fidelity numerical simulations of microstructurally small phenomena".
4. **Sandia National Laboratories** – Invited seminar at Sandia Engineering Sciences Center (August 2016). Albuquerque, New Mexico. "Combining experiments, simulation, and machine learning to investigate small-crack growth mechanisms in 3D".
5. **International Union of Theoretical and Applied Mechanics** – Invited presentation at IUTAM Symposium on Integrated Computational Structure-Material Modeling of Deformation and Failure under Extreme Conditions (June 2016). Baltimore, Maryland. "Integrating data from experiments & simulations to elucidate small-crack growth mechanisms".
6. **American Society of Material (ASM) Spring Symposium** – Invited speaker at Eastern New York Chapter of ASM International Spring Symposium at GE Global Research Center (April 2016). Niskayuna, New York. "Combining experiments, modeling, and machine learning to study 3D crack propagation".
7. **Duke University** – Seminar in Department of Civil Engineering (January 2016). Durham, North Carolina. "Improving understanding and prediction of microstructurally small crack growth by coupling experimental observations, numerical simulations, and machine learning".

8. **University of Michigan** – Seminar in Department of Materials Science and Engineering (January 2016). Ann Arbor, Michigan. "Improving understanding and prediction of microstructurally small crack growth by coupling experimental observations, numerical simulations, and machine learning".
9. **Johns Hopkins University** – Seminar in Department of Civil Engineering (June 2015). Baltimore, Maryland. "Multi-scale modeling of microstructurally small fatigue cracks in an aluminum alloy from synchrotron-based measurements".

5.3 Conference Presentations Acknowledging this AFOSR YIP Award (presenter)*

1. A.D. Spear*, "A data-driven approach to predict microstructurally small fatigue-crack evolution", *TMS Annual Meeting and Exhibition*, Phoenix, Arizona, March 2018. **Invited**
2. B.R. Phung*, A.D. Spear, "A voxel-based meshing framework for the simulation of arbitrary 3D crack growth in heterogeneous materials", *TMS Annual Meeting and Exhibition*, Phoenix, Arizona, March 2018.
3. A.D. Spear*, "On the interaction of 3D crack surfaces with grain boundaries in polycrystalline materials", *Materials Research Society (MRS) Fall Meeting*, Boston, Massachusetts, November 2017. **Invited**
4. B.R. Phung*, A.D. Spear, "A voxel-based meshing framework for the simulation of arbitrary 3D crack growth in heterogeneous materials", *International Conference on Fracture (ICF 14)*, Rhodes, Greece, June 2017.
5. K.J. DeMille*, A.D. Spear, "Establishment of representative volume elements for the analysis of microstructurally small cracks in polycrystalline materials", *International Conference on Fracture (ICF 14)*, Rhodes, Greece, June 2017.
6. N. Wilkinson, K. Pierson, P.T. Fletcher, J.D. Hochhalter**,** A.D. Spear*, "Toward the use of machine learning to predict microstructurally small fatigue crack evolution", *TMS Annual Meeting and Exhibition*, San Diego, California, February 2017.
7. B.R. Phung*, B. Leavy, R. Brannon, A.D. Spear, "A comparison between the finite element method and material point method in mesoscale crystal plasticity simulations", *Engineering Mechanics Institute*, Nashville, Tennessee, May 2016.
8. A.D. Spear*, J.D. Hochhalter, A.R. Cerrone, A.R. Ingraffea, "Generation of conformal finite-element meshes from 3D measurements of microstructurally small fatigue-crack propagation", *Engineering Mechanics Institute*, Nashville, Tennessee, May 2016.
9. A.D. Spear*, J.D. Hochhalter, A.R. Cerrone, S.F. Li, J.F. Lind, R.M. Suter, A.R. Ingraffea, "Multiscale simulation of observed 3D crack evolution in a polycrystalline aluminum alloy", *13th U.S. National Congress on Computational Mechanics*, San Diego, California, July 2015.
10. A.D. Spear*, J.D. Hochhalter, A.R. Cerrone, S.F. Li, J.F. Lind, R.M. Suter, A.R. Ingraffea, "Combined multi-scale characterization and modeling of 3D fatigue-crack evolution in an aluminum alloy", *ASME Applied Mechanics and Materials*, Seattle, Washington, June 2015.

6. Project Team

The project team includes Assistant Professor Ashley Spear; graduate students Brian Phung, Karen DeMille, and Kyle Pierson of the University of Utah; and Associate Professor P. Thomas Fletcher of the Scientific Computing and Imaging Institute at the University of Utah, who co-advises Kyle Pierson. The team collaborates with Drs. Ravi Chona, Ben Smarslok, and Brian Gockel of the Structural Sciences Center at AFRL.