AFRL-RX-WP-TP-2012-0410

PROBABILISTIC FRAMEWORK FOR PREDICTION OF MATERIAL PROPERTY DISTRIBUTIONS FROM SMALL MICROSTRUCTURAL MODELS (PREPRINT)

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AUGUST 2012
Interim

AIR FORCE RESEARCH LABORATORY
MATERIALS AND MANUFACTURING DIRECTORATE
WRIGHT-PATTERSON AIR FORCE BASE, OH 45433-7750
AIR FORCE MATERIEL COMMAND
UNITED STATES AIR FORCE

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

1. REPORT DATE *(DD-MM-YY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
August 2012	Technical Paper	1 July 2012 – 1 August 2012

4. TITLE AND SUBTITLE
PROBABILISTIC FRAMEWORK FOR PREDICTION OF MATERIAL PROPERTY DISTRIBUTIONS FROM SMALL MICROSTRUCTURAL MODELS (PREPRINT)

5a. CONTRACT NUMBER In-house
5b. GRANT NUMBER
5c. PROGRAM ELEMENT NUMBER 62102F

6. AUTHOR(S)
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5d. PROJECT NUMBER 4349
5e. TASK NUMBER 20
5f. WORK UNIT NUMBER X05W

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Metals Branch
Structural Materials Division
2230 Tenth Street
Wright-Patterson AFB, OH 45433-7750

8. PERFORMING ORGANIZATION REPORT NUMBER
AFRL-RX-WP-TP-2012-0410

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Air Force Research Laboratory
Materials and Manufacturing Directorate
Wright-Patterson Air Force Base, OH 45433-7750
Air Force Materiel Command, United States Air Force

10. SPONSORING/MONITORING AGENCY ACRONYM(S)
AFRL/RXCM

11. SPONSORING/MONITORING AGENCY REPORT NUMBER(S)
AFRL-RX-WP-TP-2012-0410

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unlimited. Preprint to be submitted to AIAA SDM Conference.

13. SUPPLEMENTARY NOTES
This work was funded in whole or in part by Department of the Air Force In house. The U.S. Government has for itself and others acting on its behalf an unlimited, paid-up, nonexclusive, irrevocable worldwide license to use, modify, reproduce, release, perform, display, or disclose the work by or on behalf of the U.S. Government. PA Case Number and clearance date: 88ABW-2012-1617, 22 March 2012. This document contains color.

14. ABSTRACT
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15. SUBJECT TERMS
probabilistic; representative volume element (rve); multiscale modeling; extreme value theory

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT:	NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON (Monitor)
a. REPORT	b. ABSTRACT	c. THIS PAGE			
Unclassified	Unclassified	Unclassified	SAR	18	Patrick Golden
					19b. TELEPHONE NUMBER *(Include Area Code)* N/A

Probabilistic Framework for Prediction of Material Property Distributions from Small Microstructural Models

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A probabilistic framework for prediction of material property distributions from small scale (i.e. 2-grain) models is proposed. Monte Carlo Simulation and kernel density estimation are used to estimate the material property distribution of a grain boundary with a 2-grain model. Extreme value and order statistics are then employed to estimate the distribution of larger microstructure models. An example of the methodology is presented for identifying the applied uniaxial stress at which plastic slip initiates in a titanium alloy with a crystal elastic finite element model. The framework was verified by comparing the predicted plastic slip initiation strength distribution with the obtained distribution from Monte Carlo Simulation of larger scale finite element models (i.e. *n*-grain models, up to ~600 grain RVE). The methodology performs well for larger microstructure models but less so for smaller ones, for a much smaller computational cost.

Nomenclature

σ_P	=	Applied uniaxial stress necessary for plastic slip initiation
α	=	slip system index
τ_{RSS}^{α}	=	Resolved shear stress on the α^{th} slip system
τ_{CRSS}^{α}	=	Critical resolved shear stress of the α^{th} slip system
n_j^{α}	=	Slip plane normal unit vector of the α^{th} slip system
b_j^{α}	=	Slip direction unit vector of the α^{th} slip system
$F(\sigma_P)$	=	Cumulative distribution function of σ_P of the 2-grain model (parent distribution)
N	=	Number of grains neighboring a grain of interest
$F_{1:N}(\sigma_P)$	=	Cumulative distribution function of σ_P of the weakest pair of grains in a collection of N pairs
n	=	Number of grains in a model
$F_{r:n}(\sigma_P)$	=	Cumulative distribution function of σ_P of the weakest grain in a collection of n grains

I. Introduction

THE focus of much of the recent research in computational materials has been in digital representation of microstructures, constitutive relationships of different microstructural features, and multiscale modeling.[1] An important aspect of multiscale modeling is the development of a representative volume element (RVE), a volume of the microstructure of a large enough size that the distribution of the response of interest (i.e. yield strength) is in

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agreement with the distribution of the macroscopic material response. Determining the size of the RVE for a given response has been the focus of much research. Often the size of the RVE is too large to be computationally tractable for property identification. For this reason, statistical volume elements (SVEs) were developed. The SVE is smaller in general than the RVE, but is sampled many times to build up the statistics that would be captured by the RVE.[2] A natural question that arises concerning the SVE is: How small can an SVE be with minimal effect on the accuracy of the predicted macroscopic material property distribution? The smallest an SVE (measured in number of grains) could be is that of a single grain. This SVE would not include any effects on the response due to grain boundaries and as such is only suitable for modeling single crystals. The next simplest microstructure is that of 2 grains – a bicrystal. For some macroscopic material properties of interest, can a collection of 2-grain SVEs be used to build up the macroscopic distributions? This work describes a probabilistic framework that attempts to obtain such macroscopic property distributions from small 2 grain SVEs.

The property of interest in this study is the plastic initiation strength of the material. For a given applied uniaxial load, if any slip systems are activated at any location in the material, plastic slip has initiated at that location *and* the plastic slip initiation strength of the entire model has been reached. This type of behavior is called Weakest Link Theory (WLT) and has a long history of application in materials science. The statistics of WLT fall into the category of Extreme Value Theory (EVT), a subset of Order Statistics. Initially EVT was described by Weibull for characterizing the rupture of solids[3]; Batdorf revisited the concepts again for the strength of ceramics[4], and more recently Tryon and Cruse explored these concepts for fatigue life[5]. WLT is applied often in systems reliability analysis for series systems. The approach taken here in this work is to view the microstructure as a system of grains and grain boundaries, each of which have some probability of slip initiation. In the parlance of system reliability, for this study slip initiation corresponds to failure of the material, and for a given stress state, the material is either in a state of failure or survival (slip or no-slip). A concise review of order statistics and extreme value theory is given is given in subsection A. The model for slip initiation strength of a titanium alloy is presented in subsection B.

A. Order Statistics

Order statistics is concerned with the distribution of the r^{th} smallest observation in a sample of n observations. For a given sample $(X_1, X_2, \ldots X_n)$, the observations may be sorted in increasing *order* and relabeled $(X_{1:n}, X_{2:n}, \ldots X_{n:n})$. The r^{th} order statistic is the r^{th} smallest value and labeled $X_{r:n}$. The extreme values, the minimum and maximum, are then $X_{1:n}$ and $X_{n:n}$.

If the sample is random, then uncertainty in X is described by its distribution $F_P(x)$. It is given the subscript "P" to identify it as the parent distribution that determines the distributions of $X_{1:n}, X_{2:n}, \ldots X_{n:n}$. The distribution of the r^{th} order statistic is then given in terms of $F_P(x)$ as

$$F_{r:n}(x) = \sum_{k=r}^{n} \binom{n}{k} \left(F_P(x)\right)^k \left[1 - F_P(x)\right]^{n-k} = I_{F_P(x)}(r, n-r+1) \tag{1}$$

Extreme Value Theory, a subset of order statistics, gives the distribution of the minimum for r = 1 in a simpler form as

$$F_{1:n}(x) = 1 - \left(1 - F_P(x)\right)^n \tag{2}$$

B. Model of Slip Initiation in Ti-α

Ti-6Al-4V is a common alloy of titanium often used in aircraft structures and gas turbine engine components. Its high strength, low density, resistance to corrosion, and ability to withstand higher temperatures has lead to its widespread application[#]. It is categorized as an $\alpha + \beta$ alloy, and contains both the primary alpha phase and the beta phase. The alpha phase has a hexagonal close packed crystal structure (hcp) and the beta phase has a body centered cubic (bcc) crystal structure. Depending on mechanical processing and heat treatment, it presents in a microstructure ranging from fully lamellar to bi-modal to fully equiaxed, with varying volume fractions of α and β. The specific microstructure studied here is fully equiaxed. The beta phase was not modeled, so the quantitative results of this study may only correspond to microstructures with very high volume fractions of the alpha phase. The microstructure modeled is a collection of equiaxed grains made of Ti-α. Each grain has a different crystallographic orientation, as seen in Figure 1.

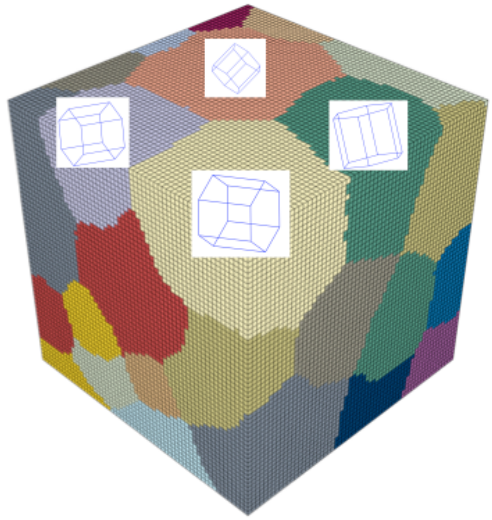

Figure 1. Fully Equiaxed Ti-6Al-4V Model – *Each grain is assigned a different crystallographic orientation. No texture was assumed.*

Each grain was assigned the same elastic material properties in the form of a stiffness tensor. The hcp Ti-α_P phase is modeled as transversely isotropic. The elasticity tensor of transversely isotropic materials has the form:

$$C_{ij} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{22} & C_{23} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{55} & 0 \\ symm. & & & & & C_{66} \end{bmatrix} \tag{3}$$

where $C_{11} = C_{22}$ and $C_{13} = C_{23}$ and $C_{55} = C_{66}$, yielding 6 independent constants that describe the elastic response of the material. The elasticity tensor selected for this study was that given in [4].

Table 1. Anisotropic Elastic Constants for Ti-α [GPa]

$C_{11} = C_{22}$	C_{33}	C_{12}	$C_{13} = C_{23}$	C_{44}	$C_{55} = C_{66}$
162.4	180.7	92.0	69.0	117	35.2

The anisotropic stiffness and varying crystallographic orientations of each grain give rise to non-uniform stresses in the microstructure, even in the presence of uniform macroscopic loading. These non-uniform stresses give rise to local plastic slip in the material.

The hcp crystal lattice has several slip system families. Slip in crystals generally occurs on planes in the lattice with relatively high close packing of atoms. These planes are called slip planes and can be specified by the vector normal to the plane. For a given slip plane, the slip occurs in a certain slip direction when the shear stress resolved on that plane in that direction exceeds the critically resolved shear stress τ_{CRSS} for that slip system. Slip systems that are identical under a rotation of the crystal lattice due to crystallographic symmetry are collected in a set called a family. The three slip system families for Ti-α_P in which plastic slip is most commonly observed are the prismatic, basal, and pyramidal. These slip systems for Ti- α_P are given in Miller-Bravais indices in Table 2 and presented in Figure 3.

Table 2. Slip Systems for Ti-α_P

Slip System Family	Slip Plane	Slip Direction
Prismatic $\{10\bar{1}0\}\langle 11\bar{2}0\rangle$	$(1\bar{1}00)$	$[11\bar{2}0]$
	$(10\bar{1}0)$	$[1\bar{2}10]$
	$(01\bar{1}0)$	$[\bar{2}110]$
Basal $\{0001\}\langle 11\bar{2}0\rangle$	(0001)	$[11\bar{2}0]$
	(0001)	$[1\bar{2}10]$
	(0001)	$[\bar{2}110]$
Pyramidal $\{10\bar{1}1\}\langle 11\bar{2}0\rangle$	$(1\bar{1}01)$	$[11\bar{2}0]$
	$(\bar{1}101)$	$[11\bar{2}0]$
	$(10\bar{1}1)$	$[1\bar{2}10]$
	$(\bar{1}011)$	$[1\bar{2}10]$
	$(01\bar{1}1)$	$[\bar{2}110]$
	$(0\bar{1}11)$	$[\bar{2}110]$

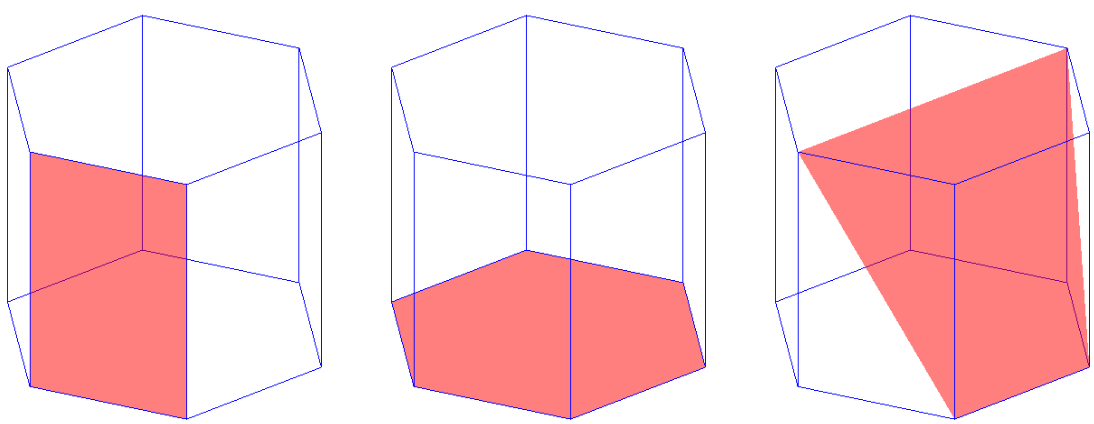

Figure 2. Prismatic, Basal, and Pyramidal Slip System Families for hcp Crystal Lattices

For the α^{th} slip system, the resolved shear stress on the slip plane with unit normal $\vec{n}$ and slip direction $\vec{b}$ is found with

$$\tau^{\alpha}_{RSS} = b^{\alpha}_i \sigma_{ij} n^{\alpha}_j \tag{4}$$

The slip plane normal and slip direction vectors are found relative to the local material coordinate system. They must be transformed into the specimen coordinate system to be implemented with the stresses from ABAQUS in the above equation.

The critically resolved shear stress for each slip system family is given in Table 3 below.

Table 3. Critically Resolved Shear Stress for Slip System Families for Ti-α_P

Slip System Family	**τ_{CRSS} [MPa]**
Prismatic	320
Basal	322
Pyramidal	846

By comparing the critically resolved shear stress with the resolved shear stress given an applied uniaxial load, the applied uniaxial load necessary for plastic slip initiation may be determined. To do so, a performance function for each slip system is developed such that when its value is less than or equal to zero, slip has initiated on that particular system.

$$g = \tau_{CRSS} - \tau_{RSS} \tag{5}$$

$$g \le 0 \quad : \quad \text{Failure (Plastic Slip Initiates)}$$
$$g > 0 \quad : \quad \text{Survival (No Plastic Slip)}$$

Assuming a linear relationship between the applied load and the value of the resolved shear stress for each slip system at every location in the microstructure

$$\tau_{RSS} = m\sigma + b \tag{6}$$

The unknowns in Eq. 7 are *m* and *b*. The results from one finite element analsyis, $\tau_{RSS} = m\sigma + b$ can be combined with the assumption that all of the resolved shear stresses are zero when the applied uniaxial stress is zero, $0 = m(0) + b$. It is then evident that the intercept *b* is zero and the slope $m = \frac{\tau_{RSS}}{\sigma}$. The extrapolation for the slip initiation strength as shown in Figure 3 is then

$$\sigma_P = \frac{\tau_{CRSS}}{\tau_{RSS}}\sigma \tag{7}$$

This σ_P is the applied uniaxial load necessary to initiate plastic slip. A value for σ_P can be found for every location in the model and the location with the smallest value of σ_P limits the allowable uniaxial load that can be applied to the model without initiating slip. This weakest link behavior suggests application of extreme value theory.

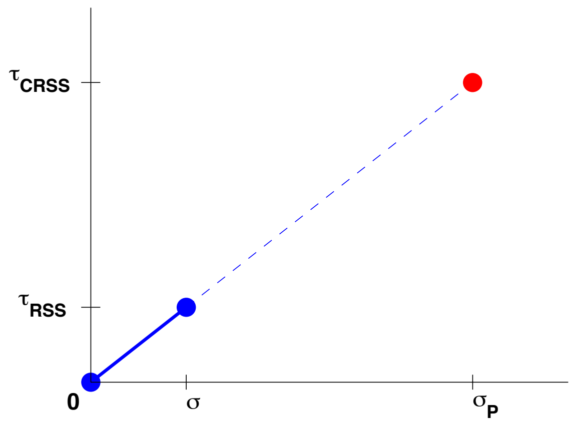

Figure 3. Extrapolation for the Uniaxial Stress Necessary to Initiate Plastic Slip on a Given Slip System – *The response τ_{RSS} is obtained from a single analysis with applied load σ. These are used to extrapolate for σ_P in which the resolved shear stress equals the critical resolved shear stress.*

The computational expense of RVE-size models prohibit the evaluation of large sample sizes for prediction of material property distributions. However, a 2-grain crystal elastic finite element model is small enough to allow the use of Monte Carlo Simulation. The uniaxial stress for plastic slip initiation may be efficiently obtained for a large number of realizations to estimate the parent distribution. The extreme value theory methodology to predict the distribution of strength of larger polycrystalline specimens is described in Section II. The results from the titanium alloy example are discussed in Section III and the conclusions are presented in Section IV. Despite the narrow scope involved with modeling only the alpha grains in a fully equiaxed microstructure, the extreme value theory framework for identifying material properties will be demonstrated. The framework can be further extended to other microstructures with appropriate modifications.

II. Methodology

The probabilistic framework developed in this work builds the distribution of the response of the macroscopic material from the distribution of the response of an SVE using order statistics. The key steps in the methodology are:

A. Sample the small-scale model with Monte Carlo simulation (MCS) to develop the distribution of the SVE response
B. Apply Extreme Value Theory and Order Statistics to estimate the distribution of the response of the large-scale model, the RVE, and hence the macroscopic material, from the SVE response distribution

Each of these steps are discussed in detail in the following subsections.

A. MCS of small-scale model for SVE response distribution

A small-scale finite element model was developed with the ABAQUS software and in this work is called an SVE. In this preliminary study, the SVE is a 2 grain or bicrystal microstructure. Each grain is modeled as a cube, and their shared face makes up their grain boundary. A perfect bond was assumed at the grain boundary. The pair of grains were enveloped in a third grain that was given the isotropic macroscopic material properties of alpha titanium to approximate the constraints on the grains that would occur in a full microstructure. The model was meshed with a grid of 20x30x40 elements. The geometry is presented below in Figure 4.

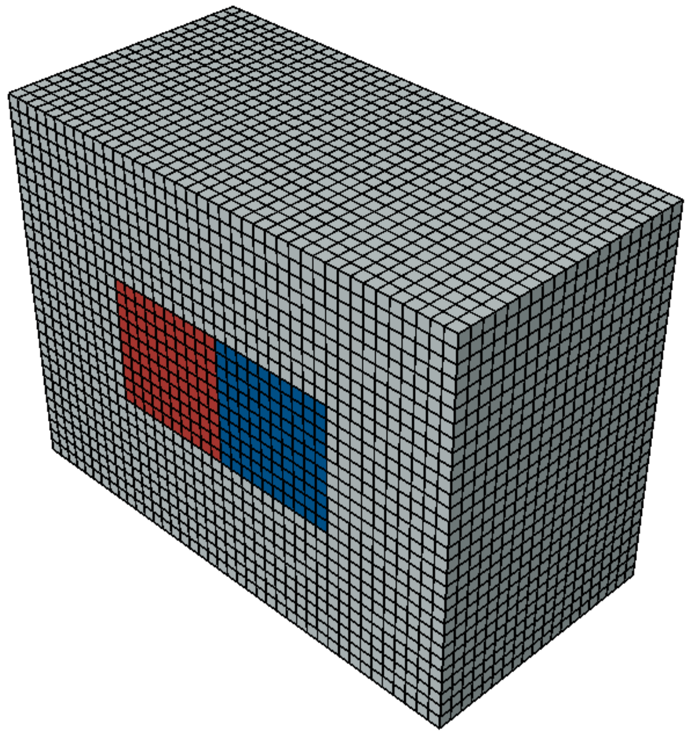

Figure 4. SVE Geometry – *The anisotropic grains are red and blue, the isotropic material is gray.*

Monte Carlo simulation (MCS) is performed with the small-scale model and the distributions of the input variables: the crystallographic orientation of each grain. For each sample, a random rotation was applied to the material orientation of each grain to generate that grain's crystallographic orientation using unit quaternions[6]. The sampling routine is included here for completeness.

1. Sample three uniform random variables: $u_1,\ u_2,\ u_3 \sim \mathrm{U}[0,1]$
2. Compute the quaternion: $q = (\beta_0, \beta_1, \beta_2, \beta_3)$

$$\beta_0 = \sqrt{1-u_1} \cdot \sin(2\pi u_2)$$

$$\beta_1 = \sqrt{1-u_1} \cdot \cos(2\pi u_2)$$

$$\beta_2 = \sqrt{u_1} \cdot \sin(2\pi u_3)$$

$$\beta_3 = \sqrt{u_1} \cdot \cos(2\pi u_3) \qquad \text{(8a,b,c,d)}$$

3. Compute the associated rotation matrix, R that transforms a coordinate in the local material coordinate system to one in the global specimen coordinate system.

$$R = \begin{bmatrix} \beta_0^2 + \beta_1^2 - \beta_2^2 - \beta_3^2 & 2(\beta_1\beta_2 + \beta_0\beta_3) & 2(\beta_1\beta_3 - \beta_0\beta_2) \\ 2(\beta_1\beta_2 - \beta_0\beta_3) & \beta_0^2 - \beta_1^2 + \beta_2^2 - \beta_3^2 & 2(\beta_2\beta_3 + \beta_0\beta_1) \\ 2(\beta_1\beta_3 + \beta_0\beta_2) & 2(\beta_2\beta_3 - \beta_0\beta_1) & \beta_0^2 - \beta_1^2 - \beta_2^2 + \beta_3^2 \end{bmatrix} \qquad (9)$$

4. The unit vectors that define the coordinate system of the material in the global coordinate system are then:

$$\{u_{sx}\} = [R]\{u_{mx}\} \Rightarrow \begin{Bmatrix} x_{sx} \\ x_{sy} \\ x_{sz} \end{Bmatrix} = [R]\begin{Bmatrix} 1 \\ 0 \\ 0 \end{Bmatrix}$$

$$\{u_{sy}\} = [R]\{u_{my}\} \Rightarrow \begin{Bmatrix} y_{sx} \\ y_{sy} \\ y_{sz} \end{Bmatrix} = [R]\begin{Bmatrix} 0 \\ 1 \\ 0 \end{Bmatrix} \tag{10}$$

$$\{u_{sz}\} = [R]\{u_{mz}\} \Rightarrow \begin{Bmatrix} z_{sx} \\ z_{sy} \\ z_{sz} \end{Bmatrix} = [R]\begin{Bmatrix} 0 \\ 0 \\ 1 \end{Bmatrix}$$

These vectors are used in ABAQUS to assign the material coordinate systems. The next step was to obtain the response of the model for each sample.

The linear elastic finite element analysis was performed for each sample to obtain the stress state, σ_{ij}, at each integration point in the model. It is assumed that plastic slip would first initiate at the grain boundary because of the discontinuity in the material properties, and thus only the integration points in elements along the grain boundary were considered. The stess tensor of the integration points along the grain boundary were used to calculate the resolved shear stress on each of the slip systems for primary alpha titanium. This was then compared with the critically resolved shear stress for each slip system. An example of the stresses is given in Figure 5.

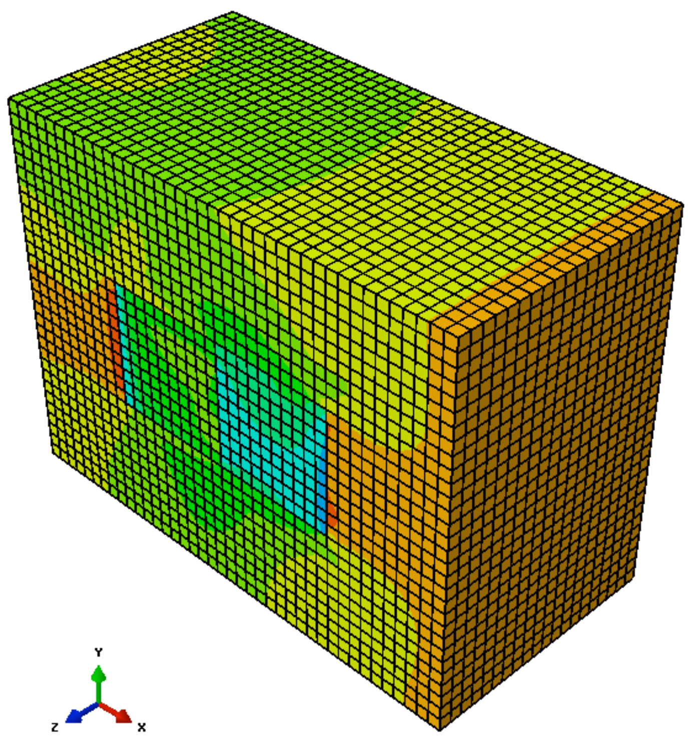

Figure 5. Example SVE Stresses σ_{xx} – *Only the stresses along the grain boundary are used in the slip initiation analysis. A uniaxial stress was applied on and normal to the near face on the right.*

The slip initiation strength was taken as the smallest uniaxial load necessary to activate any slip system at any integration point in the model. With a large sample size, kernel density estimation is then used to obtain the distribution of the slip initiation strength of a bicrystal.

B. Estimate RVE response distribution with Order Statistics and SVE response distribution

Development of the RVE response distribution is facilitated by the application of order statistics and the SVE response distribution.

The distribution of the slip initiation strength of a bicrystal is obtained in the previous step. This 2-grain distribution is then used as an approximation of the slip initiation strength for an arbitrary pair of neighboring grains in the bulk material. The key assumption made in this methodology is that the bicrystal distribution is a good approximation of the distribution of the behavior of neighboring grains in the bulk material.

Based on this approximation, the SVE distribution is then the parent distribution for use with extreme value and order statistics to develop the distribution of the slip initiation strength of the RVE. The parent distribution is denoted by its CDF, $F_P(\sigma_P)$.

The distributions for order statistics and EVT given in equations 1 and 2 are for the case where the *n* samples are independently and identically distributed. Applying these equations to the distribution of the initiation strength of different grains in an SVE will introduce some bias because the strength distribution of one grain depends on the same factors that also effect other neighboring grains (i.e. Schmid Factor) and their distributions are not independent. It is not clear how much bias is introduced by making the independence approximation. The verification tests may shed light on this issue, and even indicate if the proposed methodology can at least provide a bound on the response distribution.

1. Application of Order Statistics to determine the RVE slip initiation strength distribution from the SVE slip initiation strength distribution

Given the parent distribution (i.e. the SVE slip initiation strength distribution CDF), $F_P(\sigma_P)$ and extreme value theory, the distribution of the slip initiation strength of a single grain with *N* adjacent grain pairs as the minimum strength of the *N* pairs and modifying Eqn. 2.

$$F_{1:N}\left(\sigma_P\right) = 1 - \left(1 - F_P(\sigma_P)\right)^N \tag{11}$$

Eqn. 11 assumes the value of *N* is deterministic. Given some grain in the material, the number of its neighboring grains, *N* is a random variable with a probability mass function[#]. An example of one is given in Figure ##.

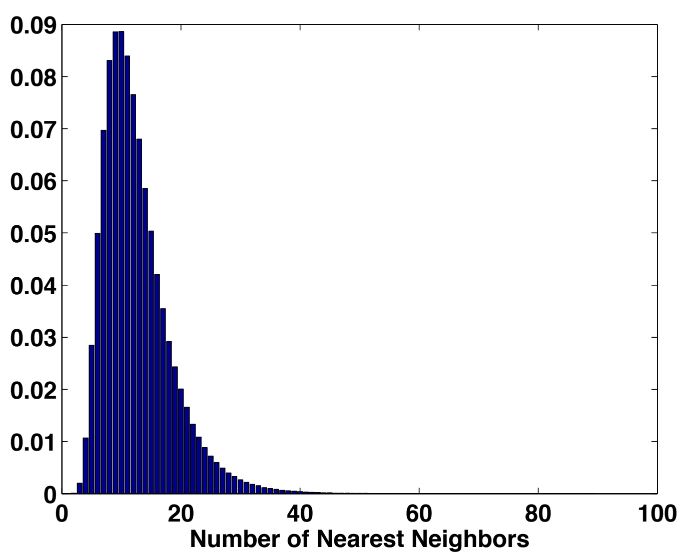

Figure 6. PMF of Number of Nearest Neighbors – *Uncertainty in the number of neighboring grains for a given grain of interest can be accounted for with the total probability theorem.*

The uncertainty in N may be addressed with the total probability theorem[#]. The total probability theorem is given by

$$P(A) = P(A|E_1)P(E_1) + \ldots + P(A|E_N)P(E_N) = \sum_N P(A|E_i)P(E_i) \tag{12}$$

Eqn. 11 is modified with Eqn. 12 to account for the uncertainty in the number of neighboring grains of a randomly selected grain with

$$F_{1:N}(\sigma_P) = \sum_{N=1}^{\max N} \left[1 - \left(1 - F_P(\sigma_P)\right)^N\right] P_N \tag{13}$$

where P_N is the probability that a grain will have N neighbors. This gives a model of the distribution of the slip initiation strength of a single grain.

Using order statistics, the applied uniaxial stress such that r independent grains in an n grain model experience slip initiation is

$$F_{r:n}(\sigma_P) = \sum_{k=r}^{n} \binom{n}{k} \left(F_{1:N}(\sigma_P)\right)^k \left[1 - F_{1:N}(\sigma_P)\right]^{n-k} = I_{F_{1:N}(\sigma_P)}(r, n-r+1) \tag{14}$$

where I is the incomplete beta function.

III. Results and Discussion

The distributions for the slip initiation strength predicted with the EVT framework for various size SVEs are presented and compared with results from MCS of SVE FE analyses .

A. Distributions predicted by 2-grain model

The 2-grain model was exercised with Monte Carlo Simulation for 200 samples. A kernel density estimate based on this data was used to obtain $F_P(\sigma_P)$. The corresponding PDF and CDF are displayed in Figure 7 below.

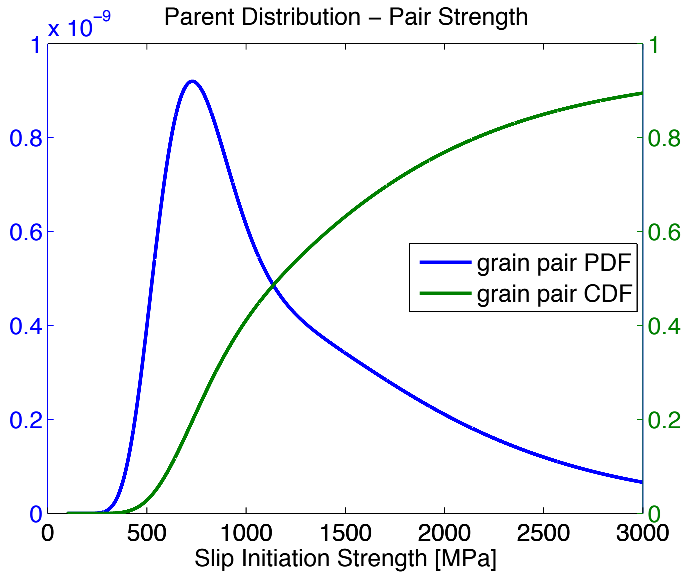

Figure 7. PDF and CDF of Slip Initiation Strength for a Random Pair of Grains Predicted by 2-grain Model – *It is assumed the 2-grain model is a good approximation of a pair of grains in a polycrystal. This "parent" distribution is used to predict the distribution for a polycrystal.*

The 2-grain parent distribution was was then used in Eq. 13 with the distribution for the nearest neighbors given in Figure 6 to obtain the distribution for the strength associated with the boundaries about a random grain. The PDF and CDF are given in Figure 8.

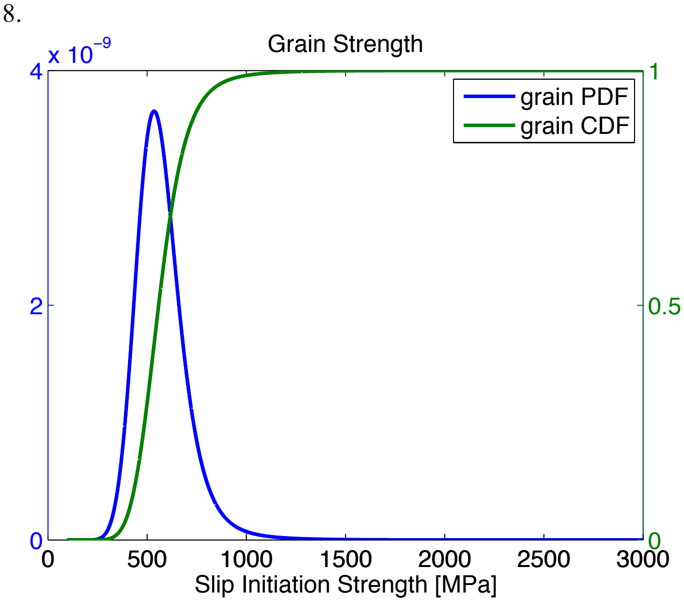

Figure 8. PDF and CDF of Slip Initiation Strength for a Random Grain Predicted by 2-grain Model – *This is the "child" distribution predicted by the 2-grain model. It is used as a "parent" distribution to predict the distribution for a polycrystal.*

The predicted grain strength distribution was then used as a parent distribution in Eq. 14 to obtain the distribution of the slip initiation strength of a polycrystal, seen in Figure 9.

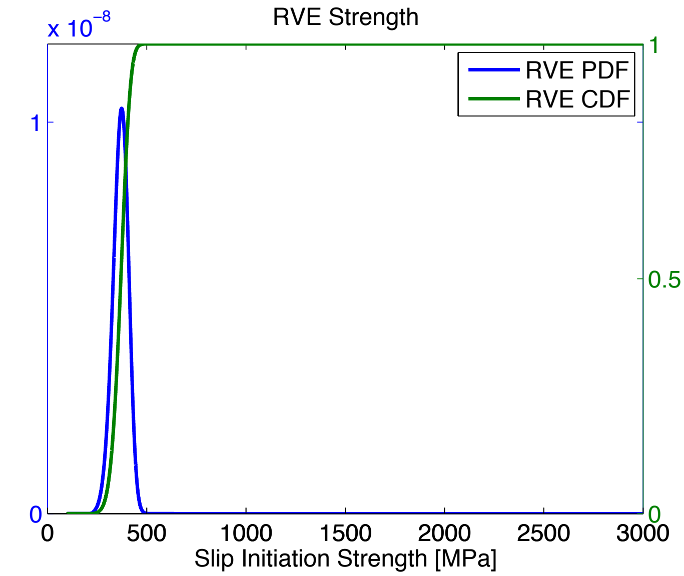

Figure 9. PDF and CDF of Slip Initiation Strength for a Polycrystal Predicted by 2-grain Model – *This is the "child" distribution of the child predicted by the 2-grain model. It was developed for a polycrystal of 30 grains.*

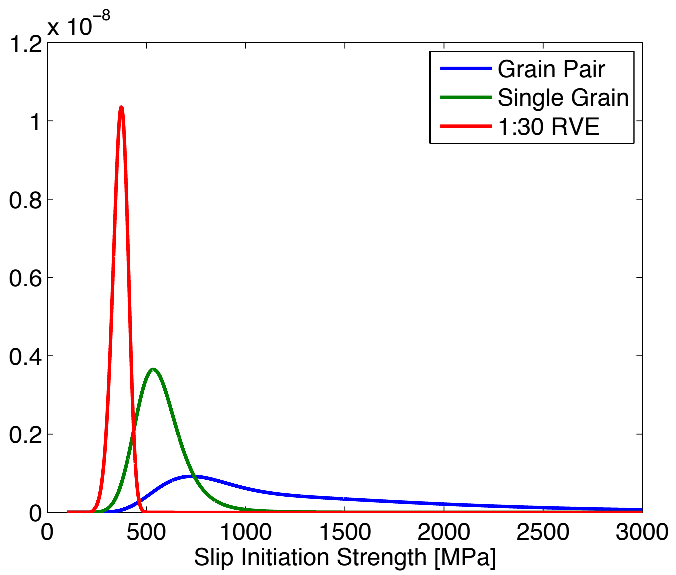

Figure 10. Comparison of Predicted Slip Initiation Strength Distributions – *The mean and variance decrease for each successive level. The predicted RVE distribution is for a polycrystal of 30-grains.*

All of the 2-grain model-predicted slip initiation strength distributions have a mean less than the macroscopic yield strength for titanium, as expected. A stronger verification of the framework was performed by running crystal elastic finite element analyses on many-grained models for comparison as described in the next section.

B. Distributions of larger SVEs

Verification tests with realizations of SVEs with more than 2 grains were performed with ABAQUS. Realizations of the statistically equivalent microstructures were generated in voxel form with DREAM.3D. The voxels were then used as brick elements in a finite element mesh for analysis with ABAQUS. Three different volumes were considered to assess the 2-grain model's prediction: 0.01x0.01x0.01 mm, 0.03x0.03x0.03 mm, and 0.1x0.1x0.1 mm.

1. ~6-grain SVE

The first verification example is shown in Figure 11a. It is a cube with side of length 0.01mm. The number of realizations generated for the verification test was 1,250. The number of grains in each realization varied as seen in Figure 11c. The mean number of grains was 5.6 grains and the standard deviation was 1.8 grains. A correlation of -0.28 was found between the extrapolated slip initiation strength and the number of grains in the SVE as seen in the scatter plot of 11d.

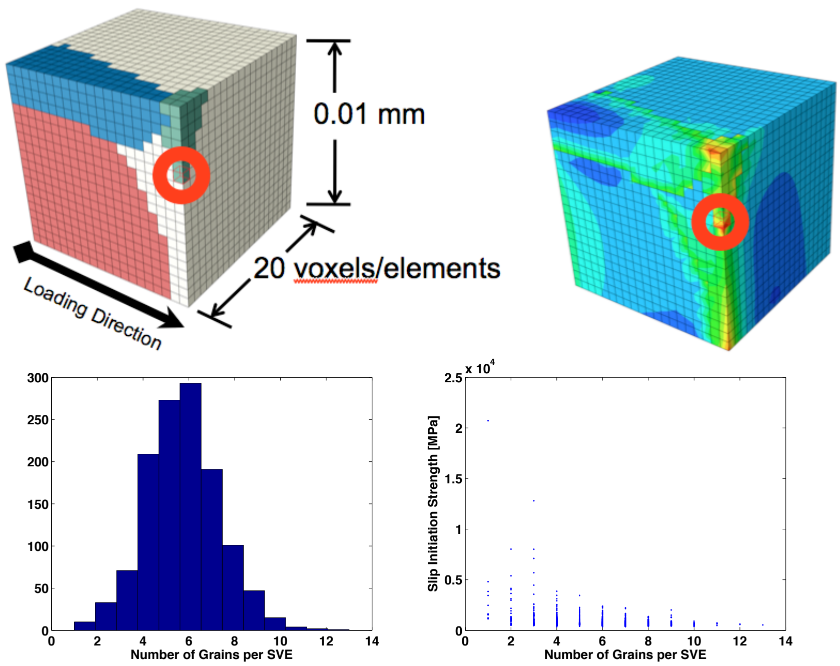

Figure 11a,b,c,&d. Example 0.01x0.01x0.01mm SVE – *A uniaxial tensile stress was applied on and normal to the front right face and the opposite face (not visible) was held fixed. The slip initiation site is enclosed by the red circle and occurred at a grain boundary for this geometry. The number of grains in each realization was random, and a small correlation (-0.28) was found between slip initiation strength and number of grains in the SVE.*

The obtained distribution of the slip initiation strength for the ~6-grain model from MCS and is presented in Figure 12a. The mean values was 900 MPa and the standard deviation was 901 MPa. The MCS distribution is compared to the predicted distribution from EVT in Figure 12b. The predicted distribution has a mean of 435 MPa and standard deviation of 94 MPa. The predicted distribution differs significantly from the actual. The lower bounds of each is similar and the predicted distribution is conservative, but the means differ by 465 MPa and the EVT predicted variance is not conservative.

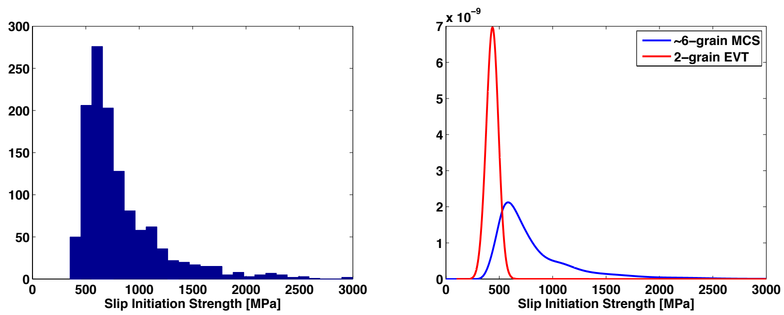

Figure 12a. MCS Distribution of Plastic Slip Initiation Strength of 0.01x0.01x0.01mm SVE – *Sample size = 1250 realizations, mean = 900 MPa, standard deviation = 901 MPa.* **b. Comparison with EVT Predicted Distribution –** *mean = 435 MPa, standard deviation = 94 MPa. The two distributions differ significantly.*

2. ~38-grain SVE

The second verification example is presented in Figure 13a and is a cube with side of length 0.03mm. The number of realizations generated for the verification test was 1,185. The number of grains in each realization varied as seen in Figure 13c. The mean number of grains was 38 grains and the standard deviation was 5.1 grains. A negligible correlation of -0.085 was found between the extrapolated slip initiation strength and the number of grains in the SVE as seen in the scatter plot of 13d.

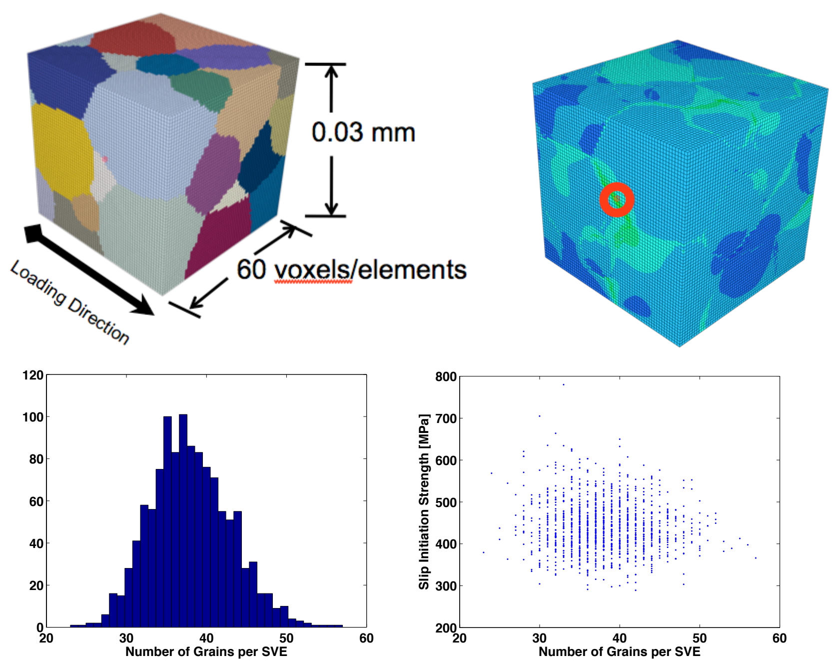

Figure 13a,b,c,&d. Example 0.03x0.03x0.03mm SVE – *A uniaxial tensile stress was applied on and normal to the front right face and the opposite face (not visible) was held fixed. The slip initiation site is enclosed by the red circle and occurred at a grain boundary for this geometry. The number of grains in each realization was random, and a neglible correlation (-0.085) was found between slip initiation strength and number of grains in the SVE.*

The obtained distribution of the slip initiation strength for the ~38-grain model from MCS and is presented in Figure 14a. The mean value was 442 MPa and the standard deviation was 61.5 MPa. The MCS distribution is compared to the predicted distribution from EVT in Figure 14b. The predicted distribution has a mean of 360 MPa and standard deviation of 37 MPa. The predicted distribution differs slightly from the actual. The lower bounds of each is similar and the predicted distribution is conservative, and the means differ by 80 MPa. However, the EVT predicted variance is not conservative.

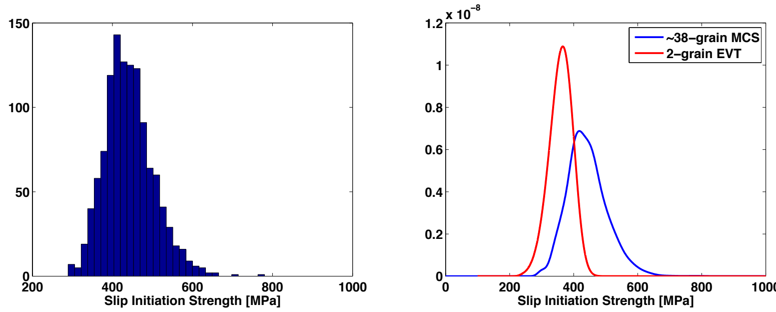

Figure 14a. MCS Distribution of Plastic Slip Initiation Strength of 0.03x0.03x0.03mm SVE – *Sample size = 1185 realizations, mean = 442 MPa, standard deviation = 62 MPa.* **b. Comparison with EVT Predicted Distribution –** *mean = 360 MPa, standard deviation = 37 MPa. The two distributions differ slightly.*

3. ~625-grain RVE

At the time of this writing, only 1 full scale model was fully analyzed for slip initiation strength. The equiaxed microstructure is shown in Figure 15. It is a cube with side of length 0.1mm and contains 625 grains. The uniaxial stress necessary to initiate plastic slip was found to be 320.5 MPa, with slip occurring on the basal plane. The EVT predicted distribution has a mean of 290 MPa and a standard deviation of 73 MPa. The mean differs from the sample point by 30.5 MPa, well within 1 predicted standard deviation.

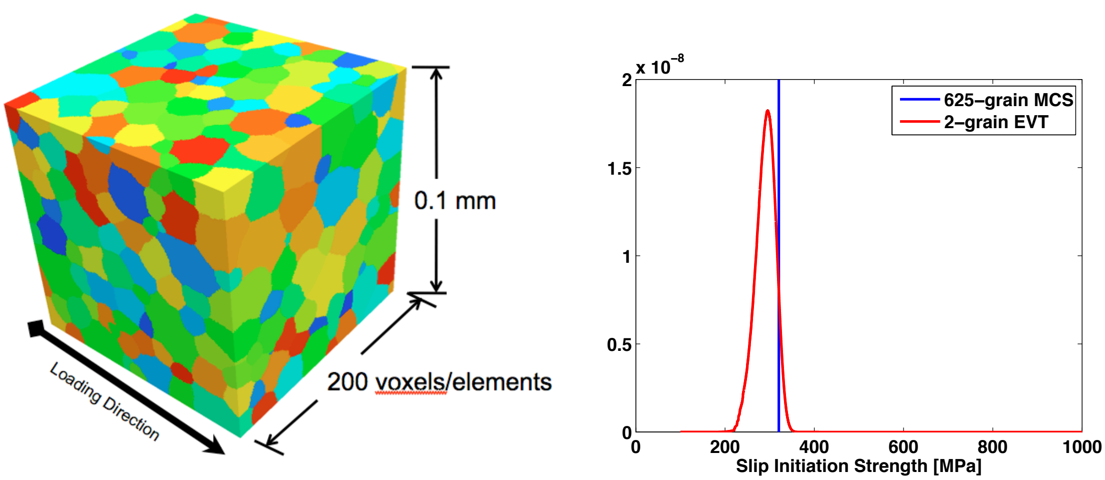

Figure 15a. Largest Model Examined, 0.1x0.1x0.1mm RVE – *A uniaxial tensile stress was applied on and normal to the front right face and the opposite face (not visible) was held fixed. Sample size = 1 realization, Slip Initiation Strength = 320.5 MPa.* **b. Comparison with EVT Predicted Slip Initiation Strength Distribution –** *mean = 290 MPa, standard deviation = 73 MPa. The EVT predicted distribution encompasses the sample point of the large scale model.*

As discussed previously, it is expected that local, microscopic yielding will take place at a lower applied uniaxial stress than that of macroscopic yielding. The range of the macroscopic yield strength of Ti-6Al-4V is ~800-1000 MPa, so the results for the large scale model fall well below the upper limit imposed by the macroscopic yield strength.

IV. Conclusion

In summary, an extreme value theory framework was presented for predicting polycrystalline model material property distributions from bicrystal model experiments. The methodology performs poorly for predicting the distribution of slip initiation strength of relatively small scale microstructure models, yet performs well for larger microstructure models. Potential causes of discrepancy between the EVT predicted distribution and the actual distribution may be due to non-local effects or the fact that grain size and shape are ignored as of this writing in the 2-grain model. Incorporating their effects may improve the ability of the proposed framework to predict material property distributions.

The successful demonstration of the proposed framework for the larger models indicates the methodology may serve as a useful technique for estimating certain material properties at a much smaller computational cost than that of exercising full large scale models.

Acknowledgments

The authors acknowledge the financial support provided by AFOSR Grant FA9550-09-1-0452, David Stargel, Program Manager. DMS expresses gratitude to Kevin Maxwell of Texas A&M for the several helpful conversations on finite element modeling. DMS acknowledges Robert Brockman of UDRI for the helpful conversations on material modeling.

References

[#]McDowell, D.L., Ghosh, S., and Kalidindi, S.R., "Representation and Computational Structure-Property Relations of Random Media," *Journal of Materials*, Vol. 63, No. 3, 2011, pp. 45-51.

[#]Przybyla, C.P., and McDowell, D.L., "Simulated microstructure-sensitive extreme value probabilities for high cycle fatigue of duplex Ti-6Al-4V," *International Journal of Plasticity*, 2011

[#]Bache, M. R., Evans, W. J., Randle, V., and Wilson, R. J., "Characterization of mechanical anisotropy in titanium alloys," *Materials Science and Engineering,* A257, 1998, pp. 139-144.

[#]Hasija, V., Ghosh, S., Mills, M., and Joseph, D., "Deformation and creep modeling in polycrystalline Ti-6Al alloys," *Acta Materialia*, Vol. 51, 2003, pp. 4533-4549.

[#]Deka, D., Joseph, D., Ghosh, S., and Mills, M., "Crystal Plasticity Modeling of Deformation and Creep in Polycrystalline Ti-6242," *Metallurgical and Materials Transactions*, 37A, 2006.

[#]Mayeur, J., and McDowell, D., "A three-dimensional crystal plasticity model for duplex Ti-6Al-4V," *International Journal of Plasticity*, Vol. 23, 2007, pp. 1457-1485

[#]Britton, T., Liang, H., Dunne, F., and Wilkonson, A., "The effect of crystal orientation on the indentation of commercially pure titanium: experiments and simulations," *Proceedings of the Royal Society A*, 466, 2010, pp. 695-917

[#]Viswanathan, G., Lee, E., Maher, D., Banerjee, S., and Fraser, H., "Direct observations and analyses of dislocation substructures in the alpha phase of an alpha/beta Ti-alloy formed by nanoindentation," *Acta Materialia*, Vol. 53, 2005, pp. 5101-5115

[#]Groeber, M., Ghosh, S., Uchic, M.D., and Dimiduk, D.M., "A framework for automated analysis and simulation of 3D polycrystalline microstructures Part 1: Statisitical characterization," *Acta Materialia*, Vol. 56, 2008, pp. 1257-1273

[#]Castillo, E., *Extreme Value Theory in Engineering*. Statistical Modeling and Decision Science, ed. G.L. Lieberman and I. Olkin. 1988, San Diego, CA: Academic Press, INC.