Modeling of Thermoelastic Stresses in Bond Coats and TBCs

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High Resolution Modeling of Materials for High Temperature Service

- **University Coal Research**: Award Number: DE-FE0003840
- *Vito Cedro*, Program Manager
- PROJECT DELIVERABLES:
  - Identify algorithm for matching both grain and particle microstructures
  - Implement and deliver software code for synthesis of digital microstructures from experimental images
  - Demonstrate that the Fast Fourier Transform (FFT) code can run as parallel (Message Passing Interface) code on a small cluster
  - Demonstrate that the FFT code can run on a large computer cluster (at least 200 nodes)
  - Characterize a candidate refractory alloy system, build the synthetic microstructure for that alloy from experimental images, perform computer simulations of mechanical response and compare computer simulations with experimental data.
  - Write and submit final report and deliver kinetic database in electronic form suitable for use by other scientists and engineers. Final report will include documentation of the 3D FFT software and the complete code for generating the synthetic microstructures and performing the mechanical response simulations

Outline

- Introduction
  - Current state of research
  - Overview of teFFT method
- Synthetic microstructure generation
  - DREAM.3D
  - Potts model interface relaxation
- Application of the teFFT code
- Extreme values: stress “hot spots”
- Summary, future work, and acknowledgments

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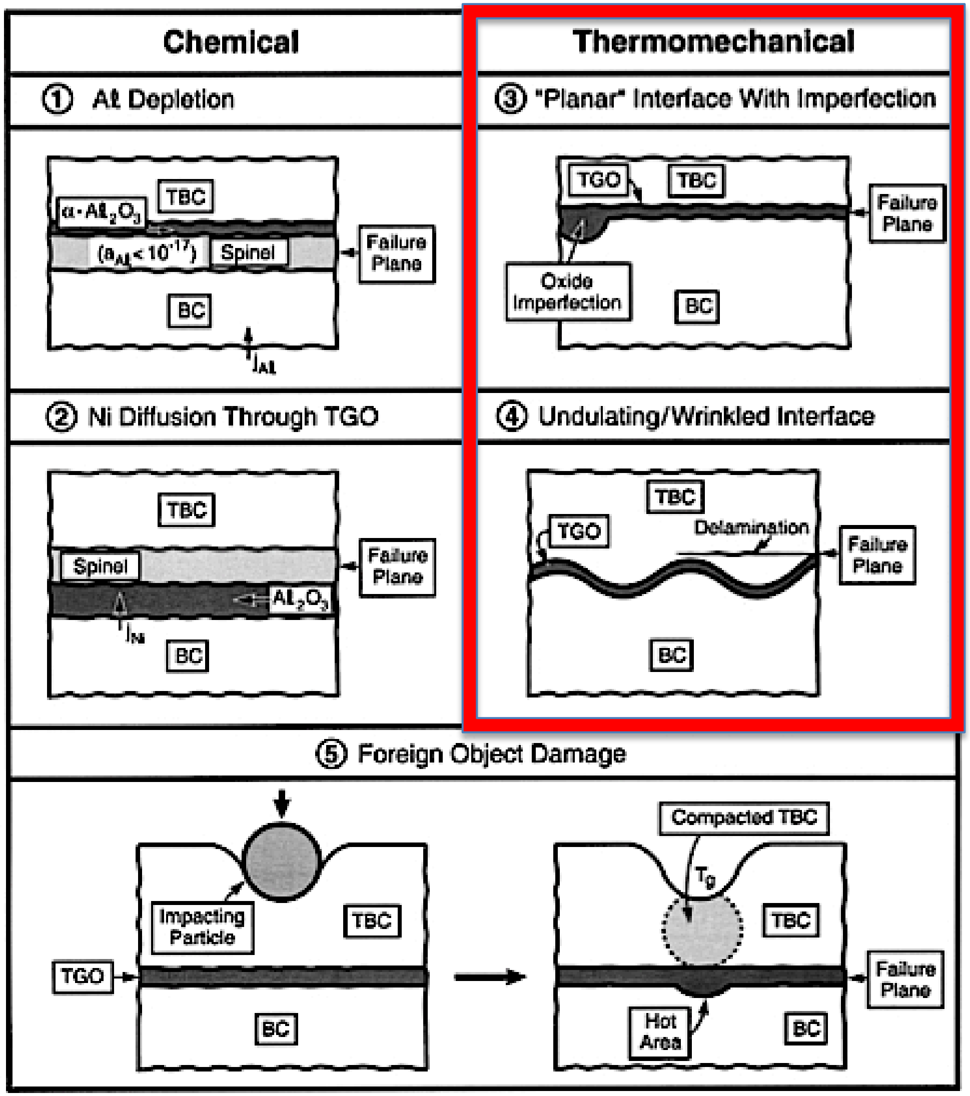
Current Research: Failure in TBC Systems

TBC failure is a complex, multi-scale problem; however, failure is most often attributed to the development of *residual stresses* at the top coat-bond coat interface.

Given a *representative microstructure*, the teFFT allows for the computation of residual stresses due to thermal expansion.

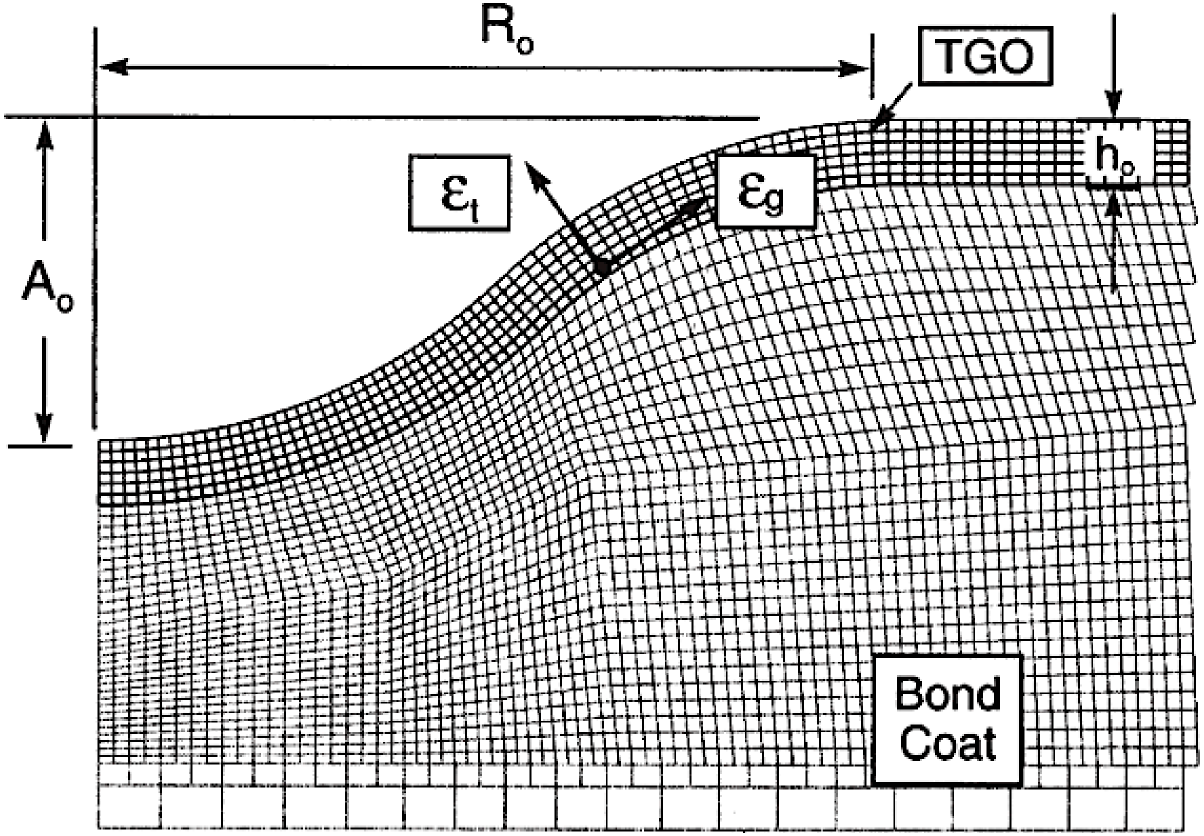


A.G. Evans, D.R. Mumm, J.W. Hutchinson, G.H. Meier, and F.S. Pettit: Prog. Mater.Sci., 2001, vol. 46, pp. 505-553.

Current Research: Modeling Techniques

Measuring thermal residual stress *in situ* is challenging; experimental techniques often cycle TBC systems to failure.

Modeling techniques such as FEM and FFT provide a non-destructive method to analyze the origins of failure.

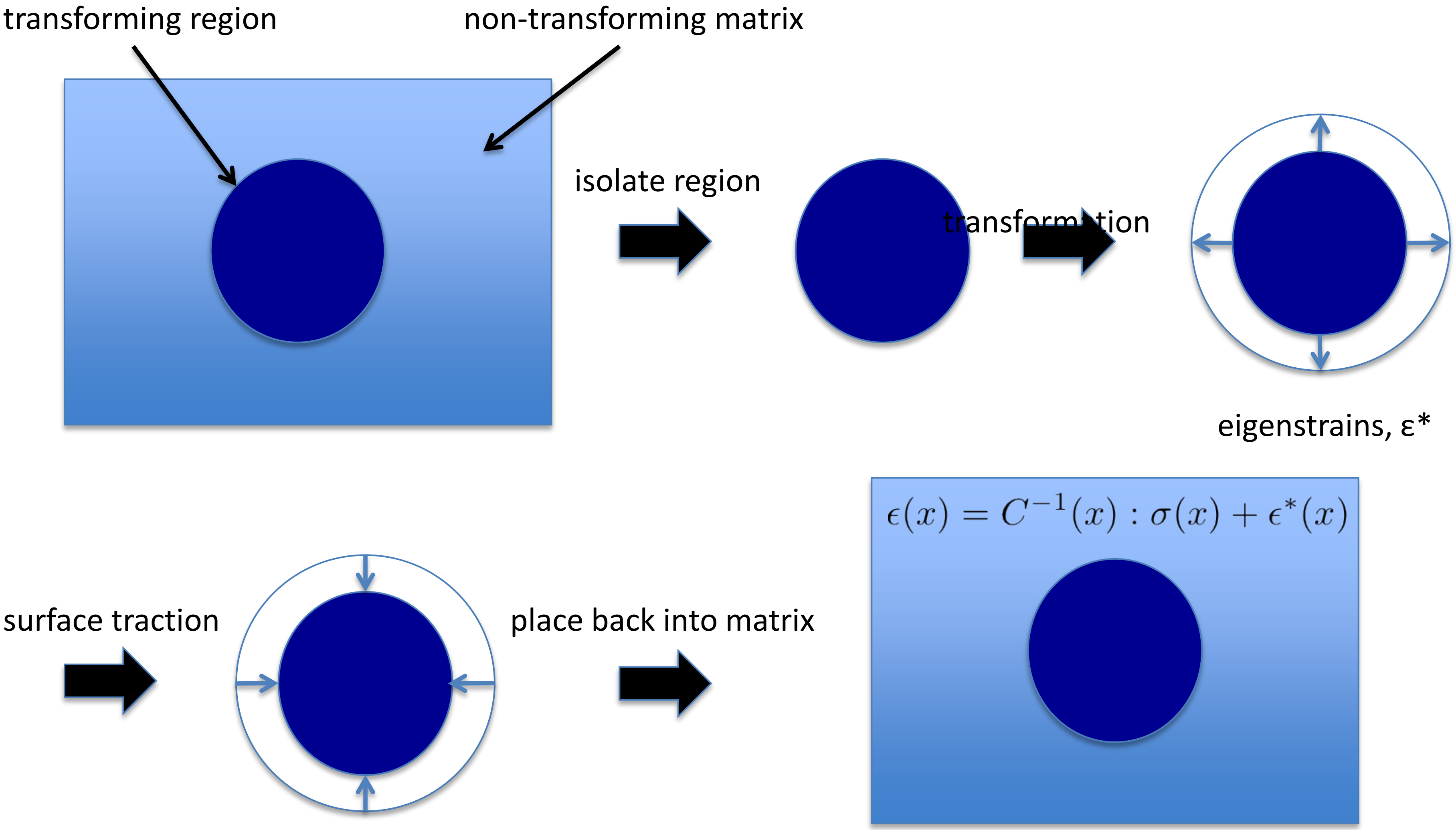


A.M. Karlsson and A.G. Evans: Acta Mater., 2001, vol. 49, pp. 1793-1804.

*F*ast *F*ourier *T*ransforms

- The FFT algorithm provides a computationally efficient way to determine direct and inverse discrete Fourier transforms.
- By re-casting PDEs in frequency space, expensive convolution integrals (Green's function method) are replaced by local (tensor) products.
- Since all calculations are local with the sole exception of the FFT, the method has the potential for *N*log*N* scaling to very large domain sizes. Parallel (MPI) schemes are readily available for FFT libraries on essentially all computer systems. It is, however, not clear that it will scale up to the exascale.
- Full field solutions to both the viscoplastic (vpFFT) and thermoelastic (teFFT) problems exist using the FFT algorithm. Both codes have been fully parallelized.
- "Eigenstrain" in this context means a stress-free strain arising from e.g. thermal expansion, e.g. phase transformation.

Eigenstrains and Eigenstresses



transforming region

non-transforming matrix

isolate region

transformation

eigenstrains, ε*

surface traction

place back into matrix

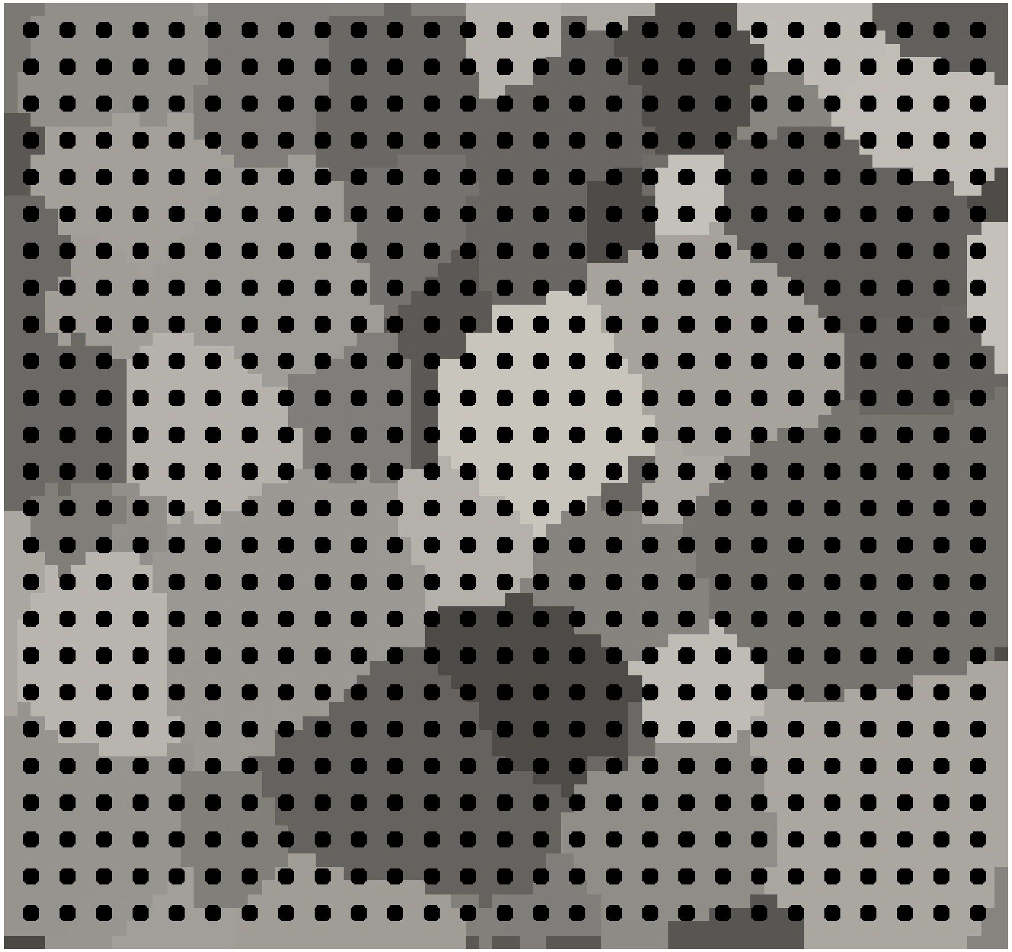
$$\epsilon(x) = C^{-1}(x) : \sigma(x) + \epsilon^*(x)$$

eigenstresses

Operation of the teFFT

We discretize the microstructure as a 3D image, or, equivalently:

A 3D regular grid is overlaid on a given representative volume element (RVE):



Each point/node contains its own information about which phase is present and the crystallographic orientation.

The teFFT algorithm computes stress and strain at each node in the grid. No additional mesh is needed.

Due to the RVE, periodic boundary conditions are required, though buffer layers can be used at the RVE boundaries.

Application of FFT to Thermoelastic Polycrystals

$$(1)\quad \varepsilon(x) = C^{-1}(x) : \sigma(x) + \varepsilon^{*}(x)$$

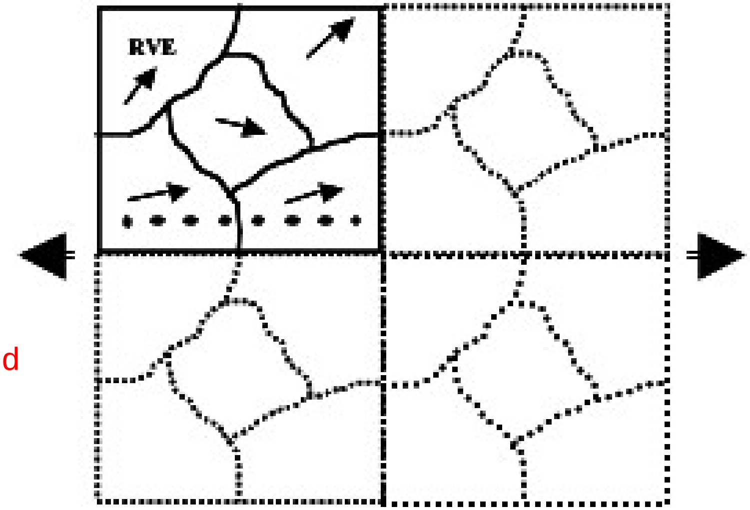
stiffness tensor of homogeneous solid

$$(2)\quad \sigma(x) = \sigma(x) + C^{o} : \varepsilon(x) - C^{o} : \varepsilon(x)$$

$$\sigma(x) = C^{o} : \varepsilon(x) + \left(\sigma(x) - C^{o} : \varepsilon(x)\right)$$

$$\sigma(x) = C^{o} : \varepsilon(x) + \tau(x)$$

perturbation in stress field



$$(3)\quad \sigma_{ij,j} = 0 \qquad \textit{in RVE}$$

$$C^{o}_{ijkl} u_{k,lj}(x) + \tau_{ij,j}(x) = 0 \qquad \textit{in RVE}$$

periodic boundary conditions in RVE

$$(4)\quad C^{o}_{ijkl} G_{km,lj}(x - x') + \delta_{im}\delta(x - x') = 0$$

$$(5)\quad \tilde{\varepsilon}_{ij}(x) = sym\left(\int_{R^3} G_{ik,jl}(x - x')\tau_{kl}(x')dx'\right) \Rightarrow \tilde{\varepsilon}_{ij} = \Gamma^{o}_{ijkl} * \tau_{kl}$$

$$\Rightarrow fft\left(\tilde{\varepsilon}_{ij} = \Gamma^{o}_{ijkl} * \tau_{kl}\right) \Rightarrow \hat{\tilde{\varepsilon}}_{ij} = \hat{\Gamma}^{o}_{ijkl} : \hat{\tau}_{kl}$$

Notation

Strain: ε

Stress: σ

Stiffness: C

Perturbation Stress: τ

Displacement: u

Green's function: G

Xformed Green's: Γ

R.A. Lebensohn: Acta Mater., 2001, vol. 49, pp. 2723-2737.

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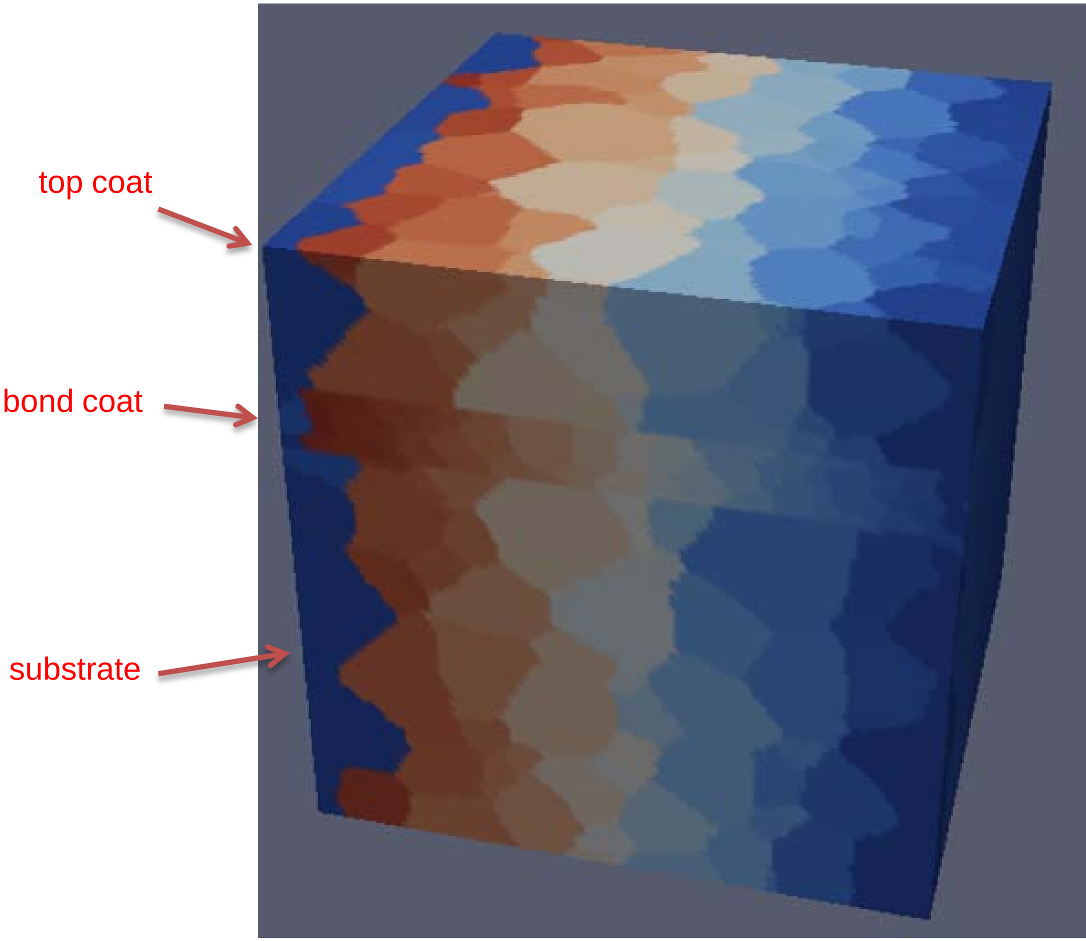
Synthetic Microstructure Generation: DREAM.3D

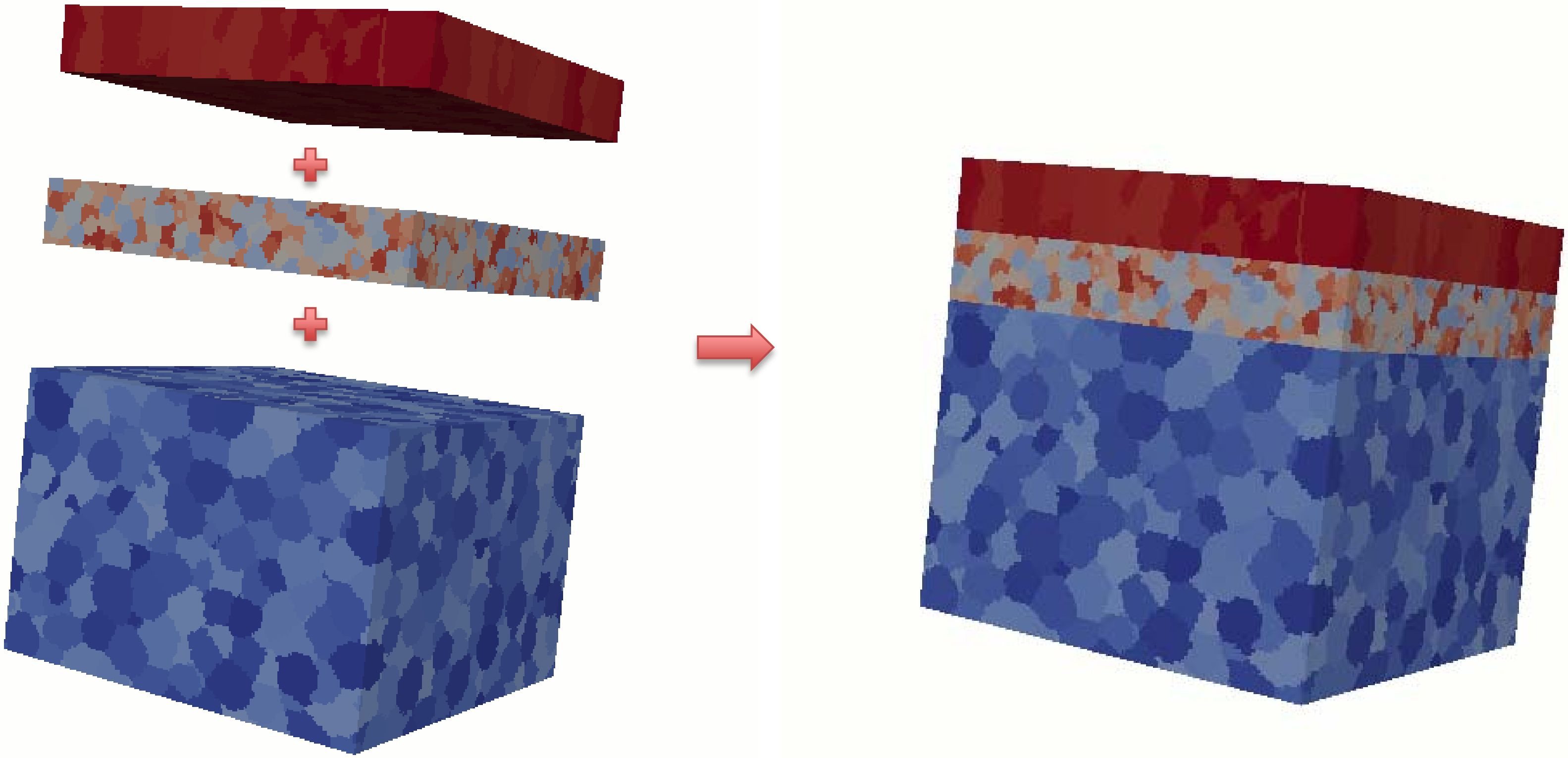
Microstructure, especially at the top coat-bond coat interface, plays a crucial role in TBC failure. To better appreciate the role of microstructure, *DREAM.3D** is used to generate test microstructures.

DREAM.3D is a tool used to generate and analyze material microstructure. DREAM.3D can create a 3D microstructure from a set of statistical data.



*available at dream3d.bluequartz.net

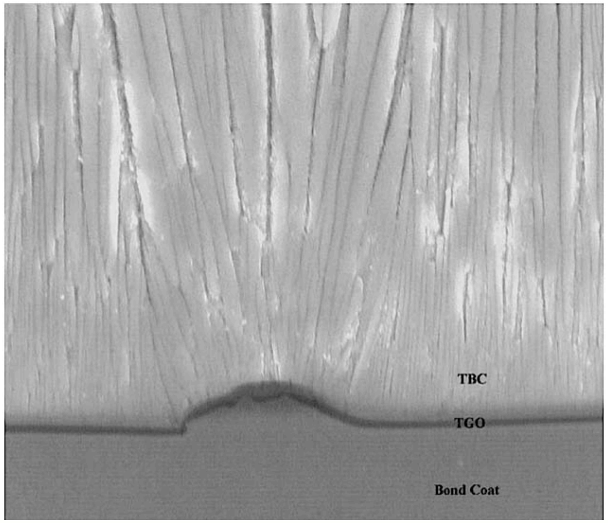
Synthetic Microstructure Generation: DREAM.3D

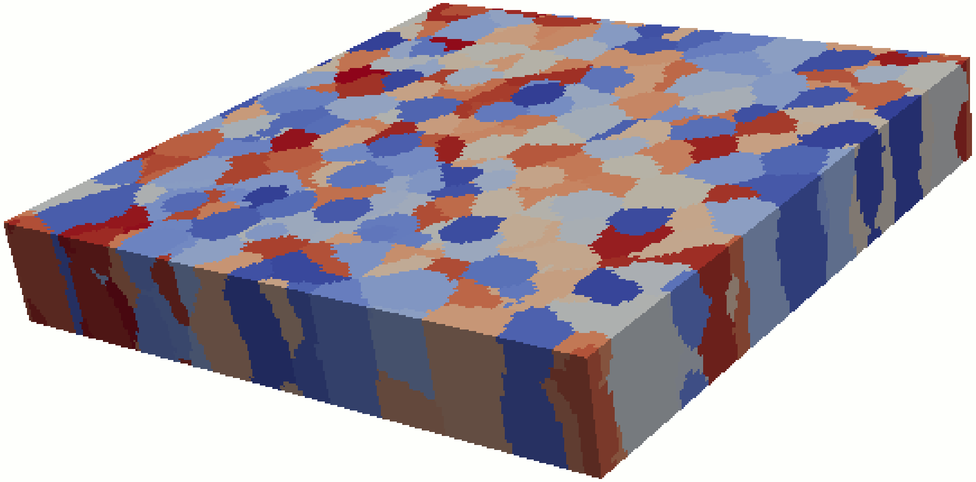


DREAM.3D is used to generate three separate microstructures representing the substrate, bond coat, and top coats in the TBC system, each with their own set of statistics and grain morphologies. The three structures are then stitched together.

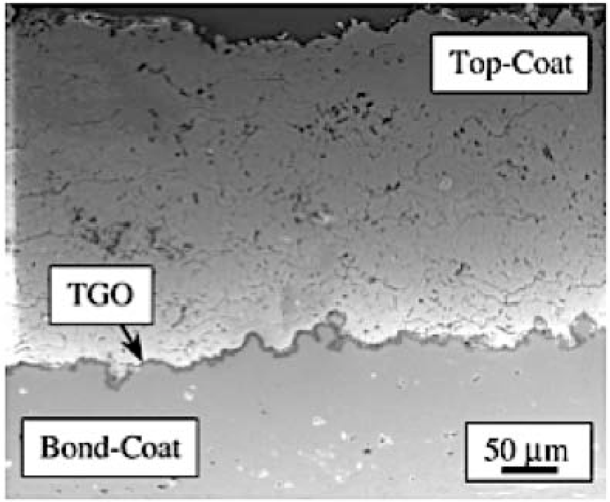
Synthetic Microstructure Generation: DREAM.3D

Top coats deposited via electron beam PVD exhibit columnar grain structures. DREAM.3D allows for the creation of such columnar grain morphologies.

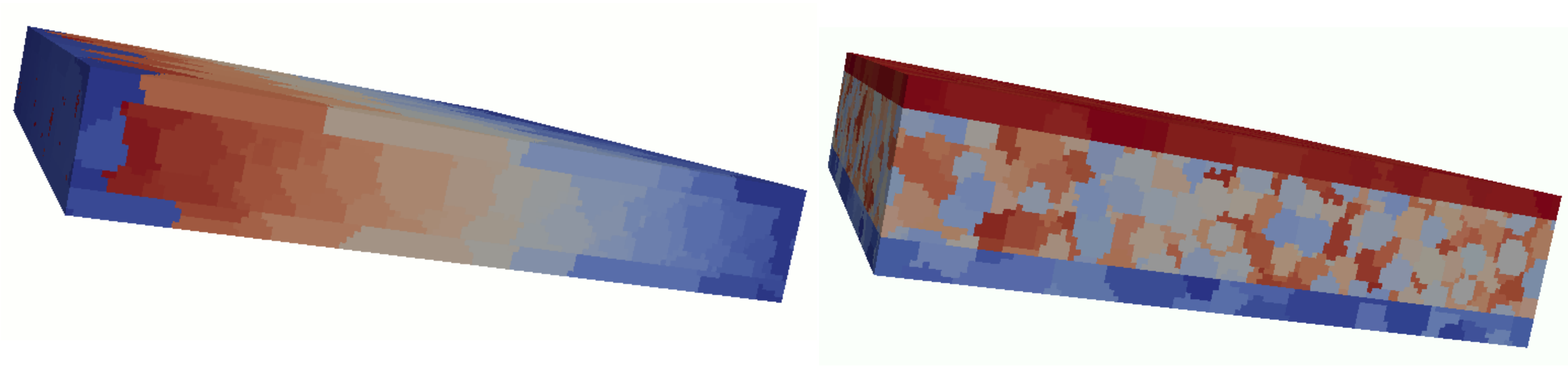




Synthetic Microstructure Generation: Interface Relaxation

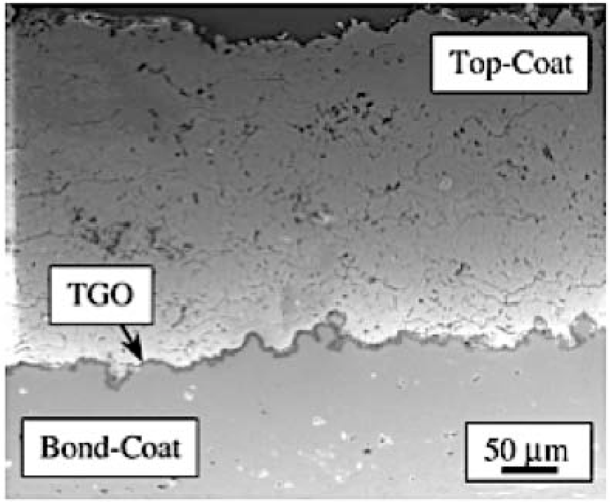


Real top coat-bond coat interfaces exhibit “undulations”. However, previous test structures did not reproduce this feature.

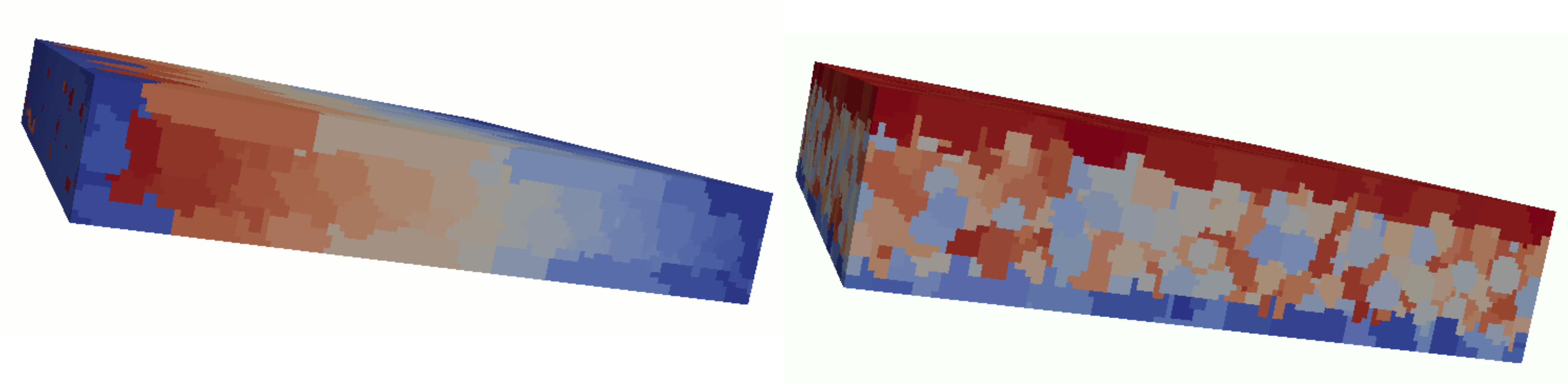


K.W. Schlichting, N.P. Padture, E.H. Jordan, and M. Gell: Mater. Sci. Eng. A, 2003, vol. 342, pp. 120-130.

Synthetic Microstructure Generation: Potts Model

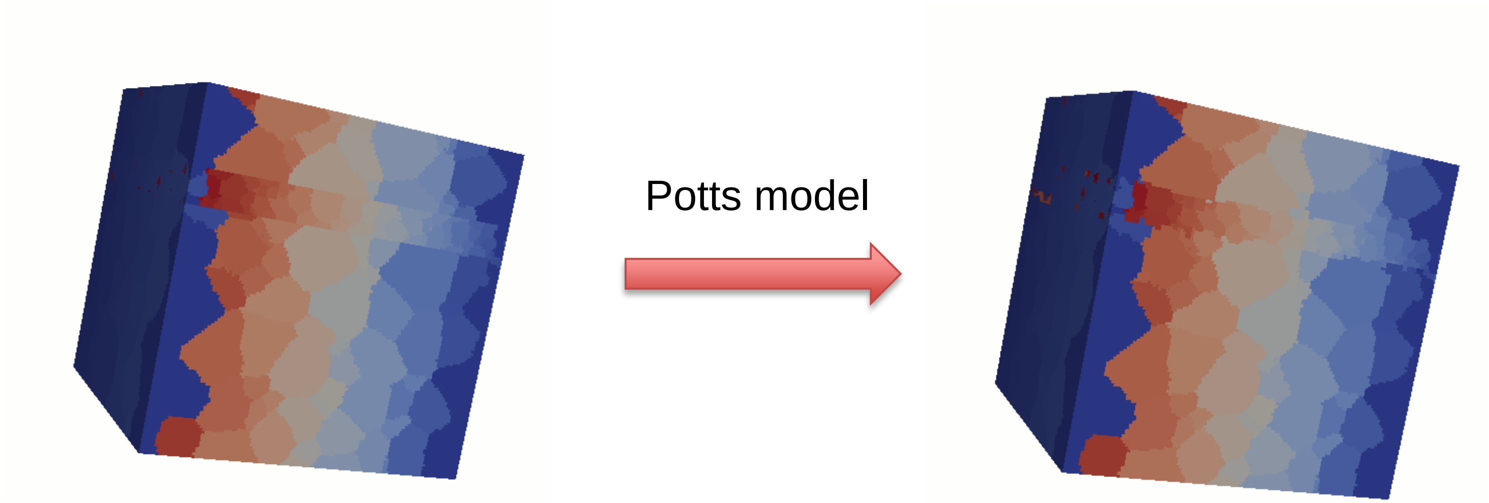


The Potts model (aka Q-state Ising model) comprises a standard isotropic grain growth model. The model is readily applied to the layers near the previously flat interfaces, allowing for ridges and undulations to naturally develop.

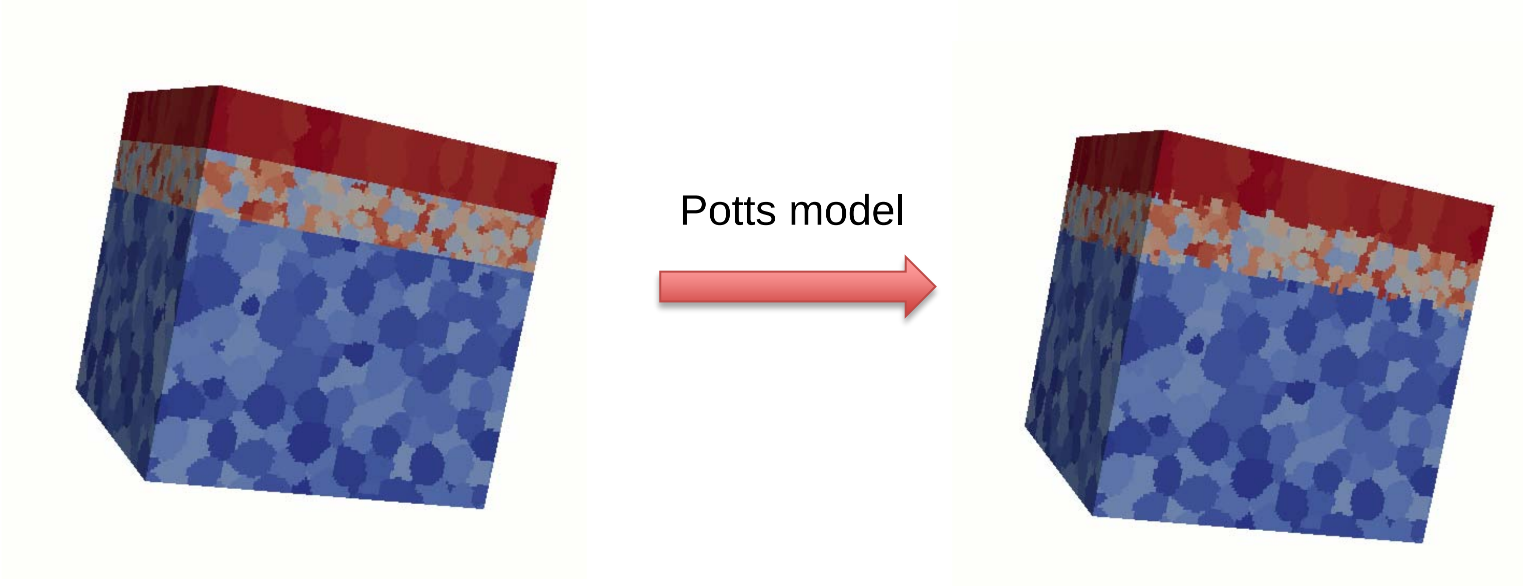


K.W. Schlichting, N.P. Padture, E.H. Jordan, and M. Gell: Mater. Sci. Eng. A, 2003, vol. 342, pp. 120-130.

Synthetic Microstructure Generation: Test Structures



Potts model



Potts model

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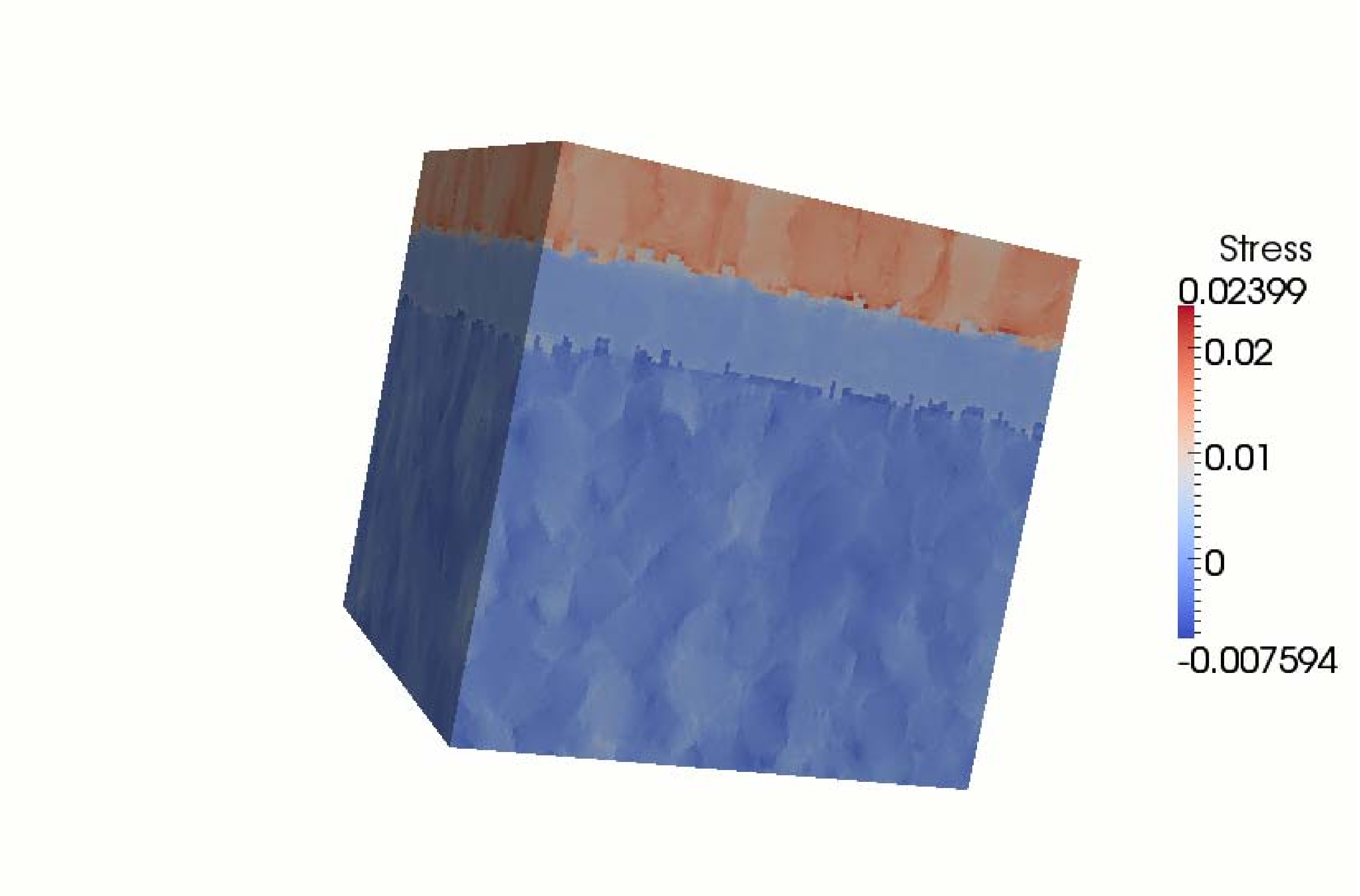
Application of the teFFT

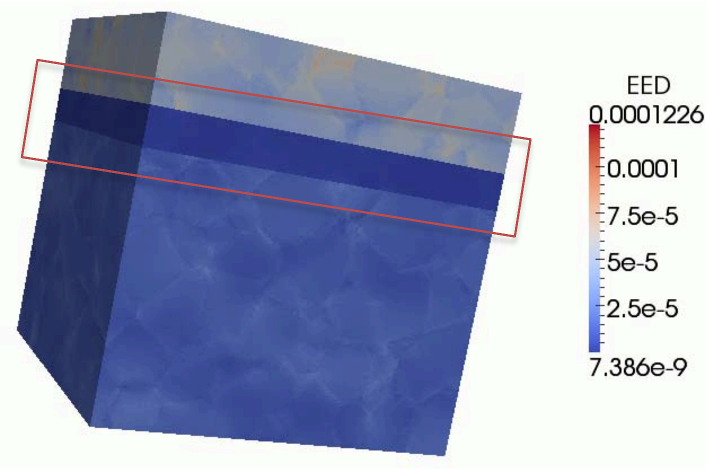
The teFFT produces full stress and strain information at each voxel in the test structure. The problem is run with a temperature change of 1000 K using industry standard materials: Inconel 718 substrate, NiCoCrAlY bond coat, YSZ top coat.

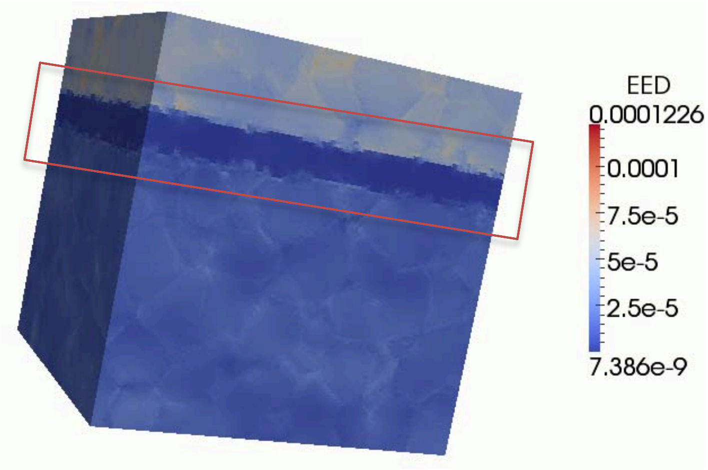


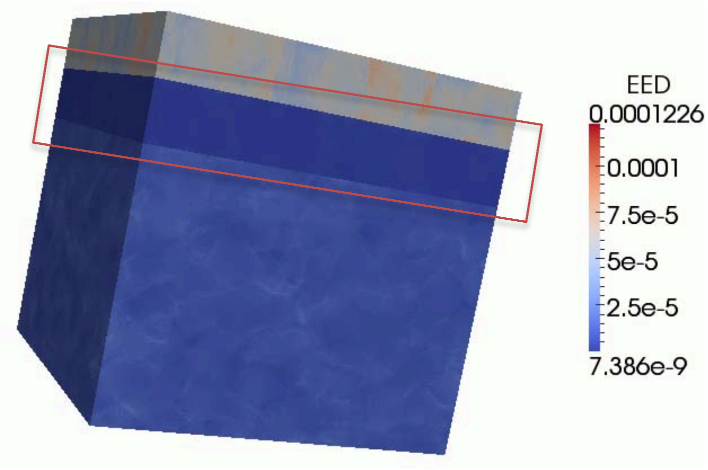
Application of the teFFT: EED

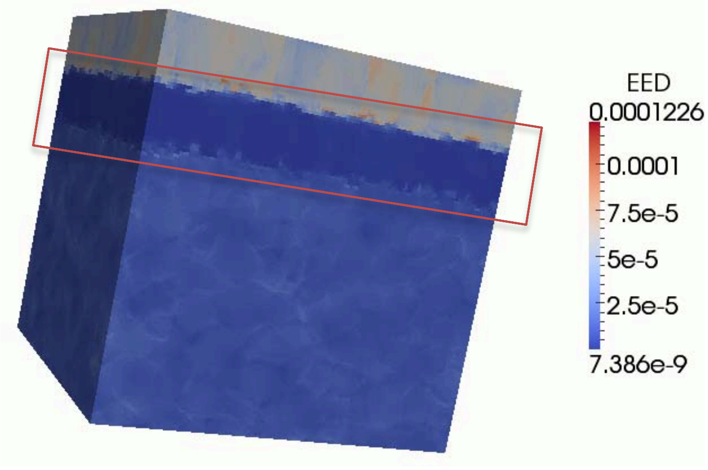
Elastic energy density (EED) provides a measure of the stored elastic energy a system, combining the information of of stress and strain.

$$EED = \frac{1}{2}\varepsilon_{ij}\sigma_{ij}$$









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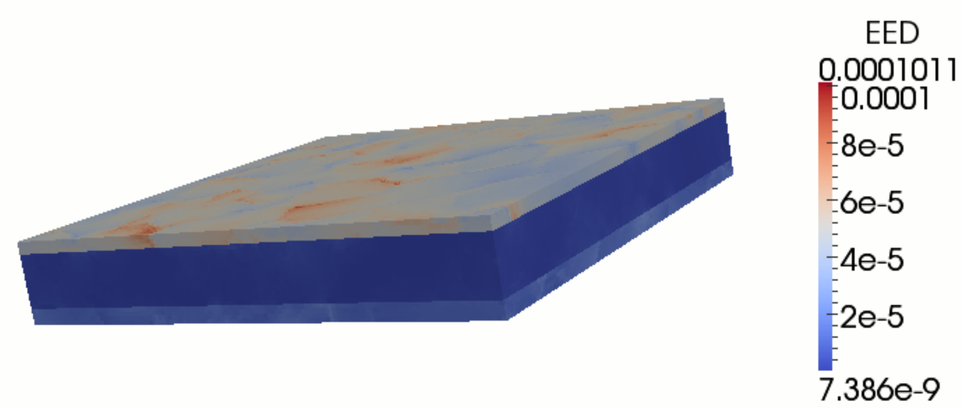
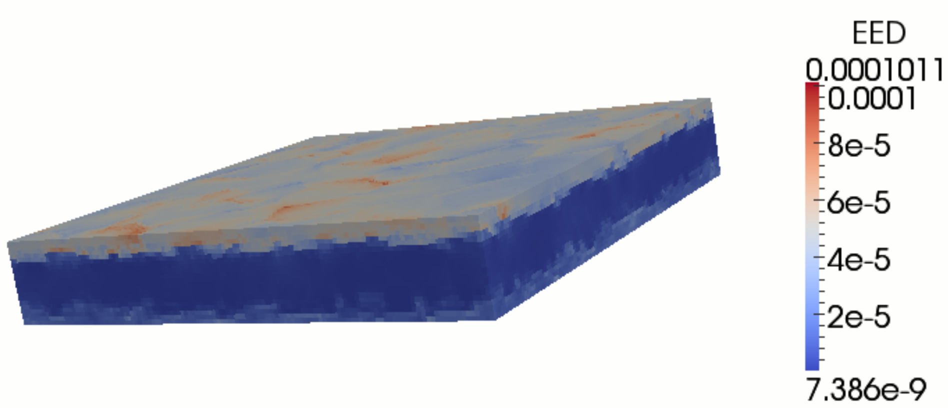
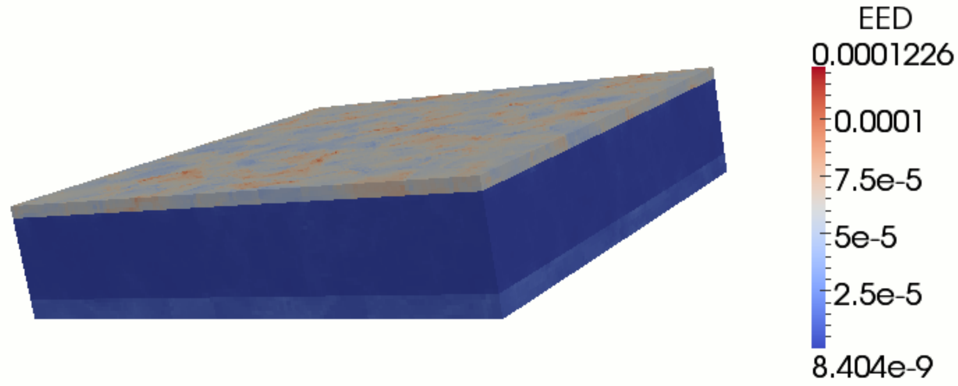
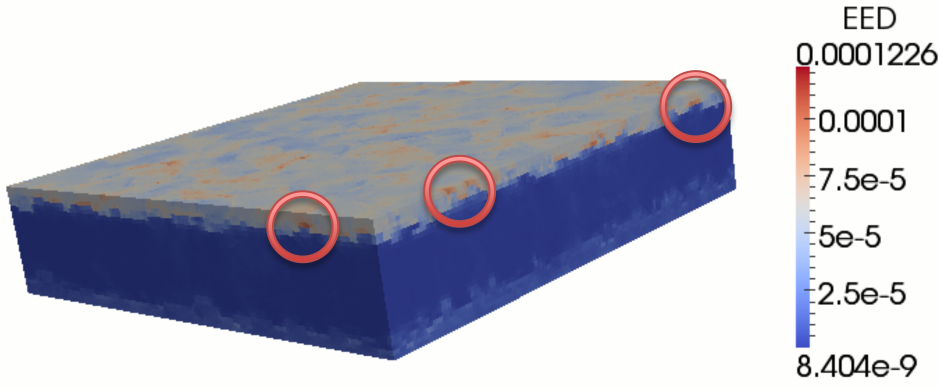
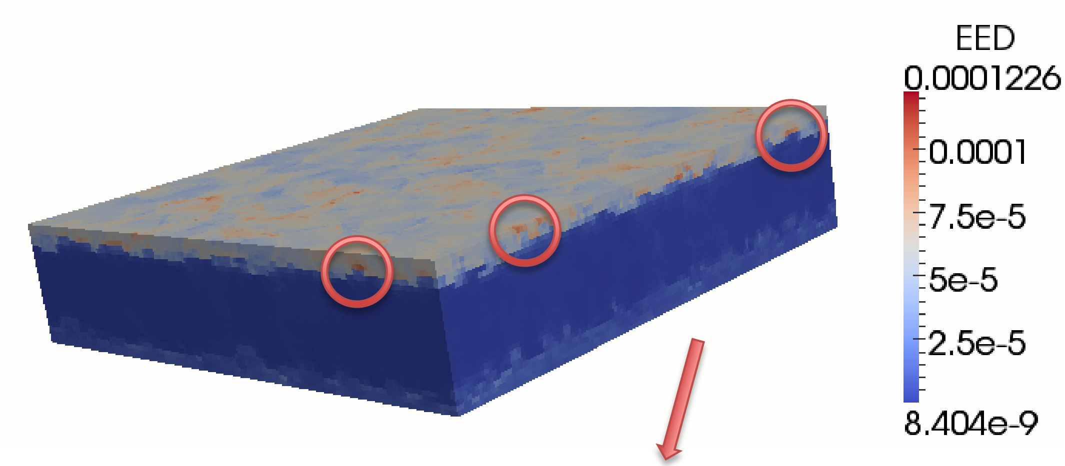




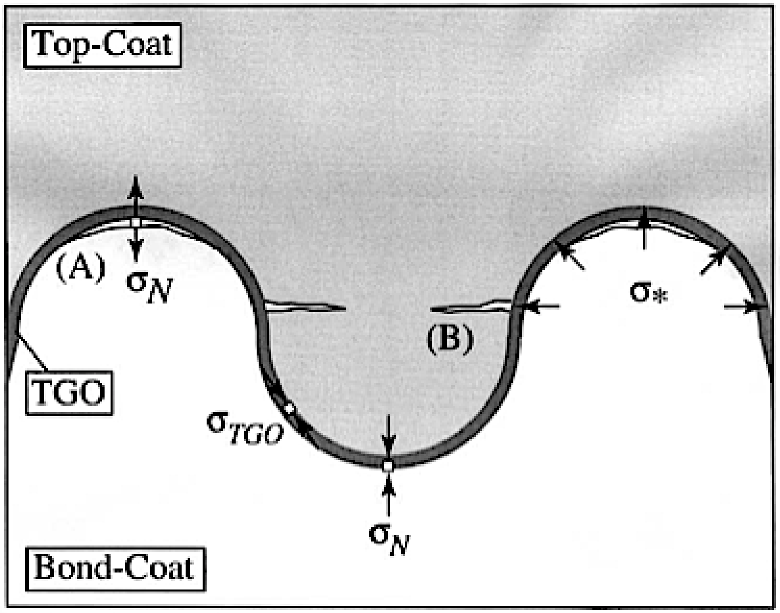


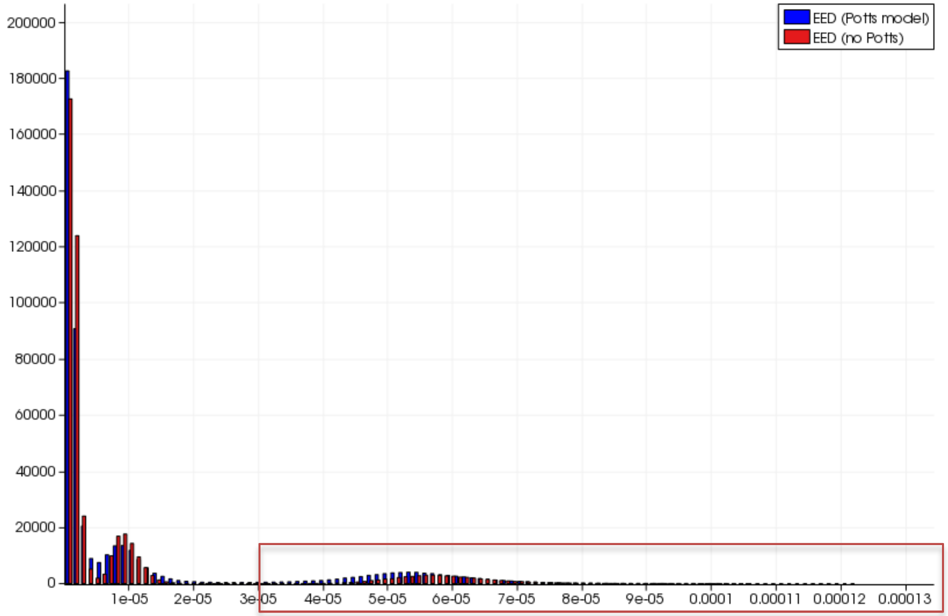


Application of the teFFT: Ridges



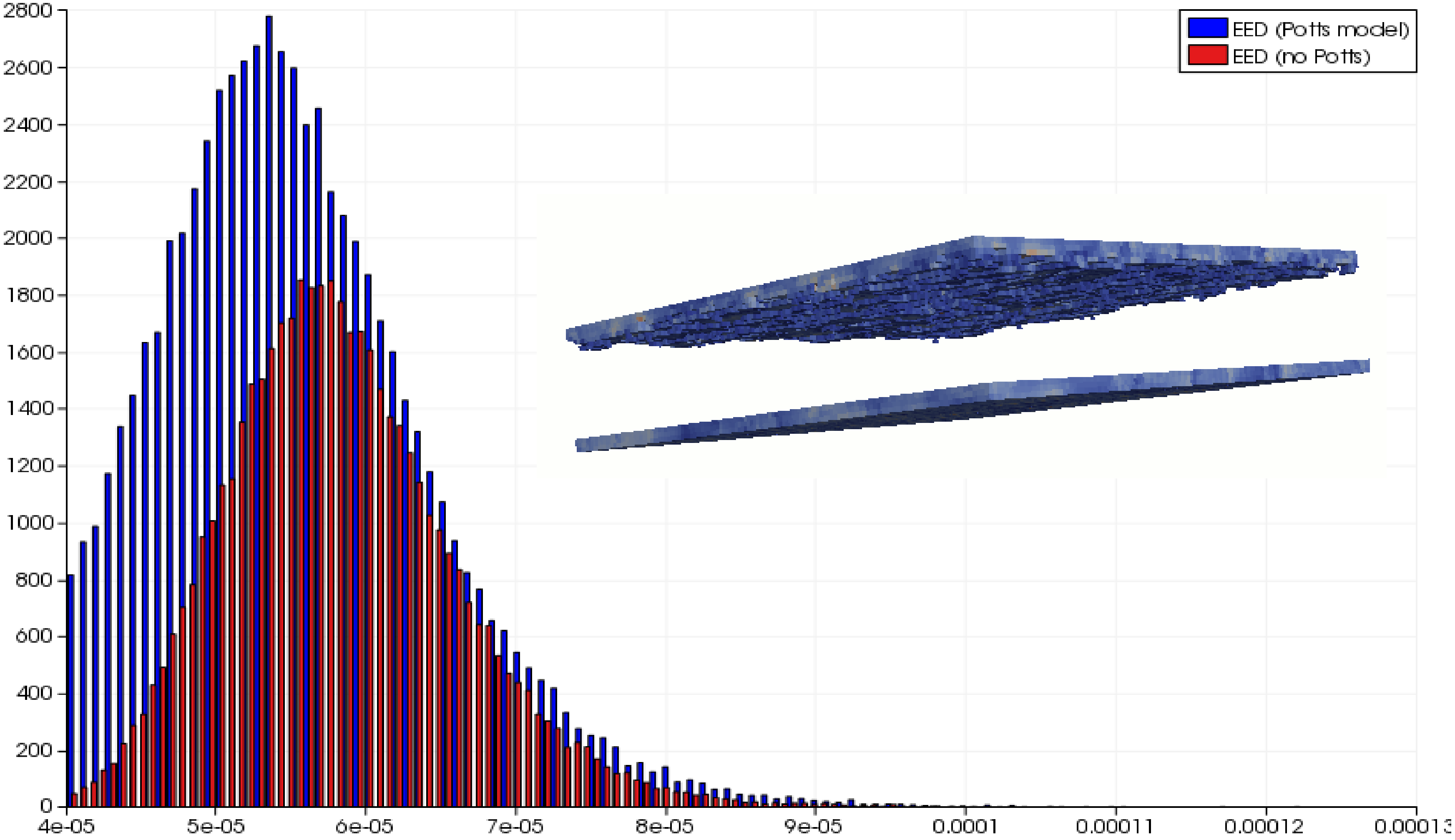
The ridges along the top coat-bond coat interface serve as points for stress concentration. Cracks preferentially nucleate near the crests of the ridges.





K.W. Schlichting, N.P. Padture, E.H. Jordan, and M. Gell: Mater. Sci. Eng. A, 2003, vol. 342, pp. 120-130.

Application of the teFFT: Thresholding by EED



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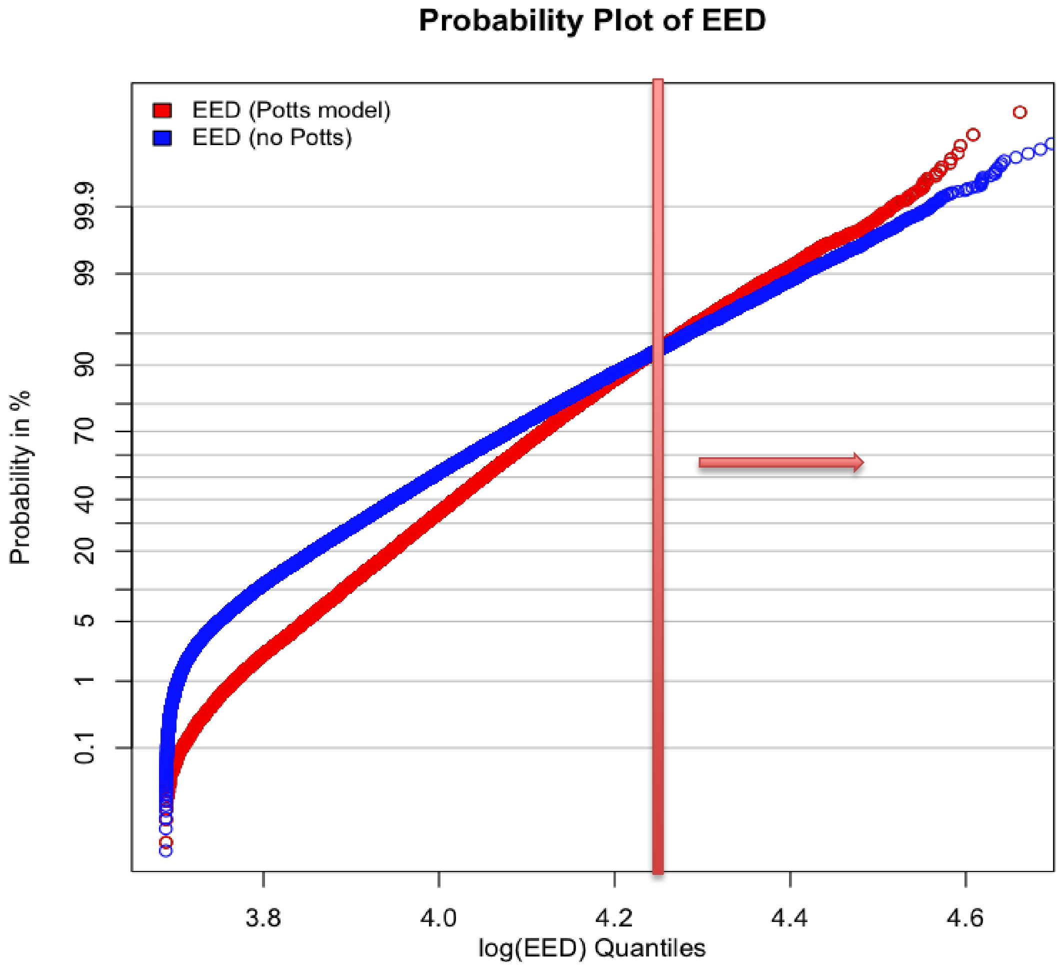
Extreme Value Analysis: Peaks over Threshold



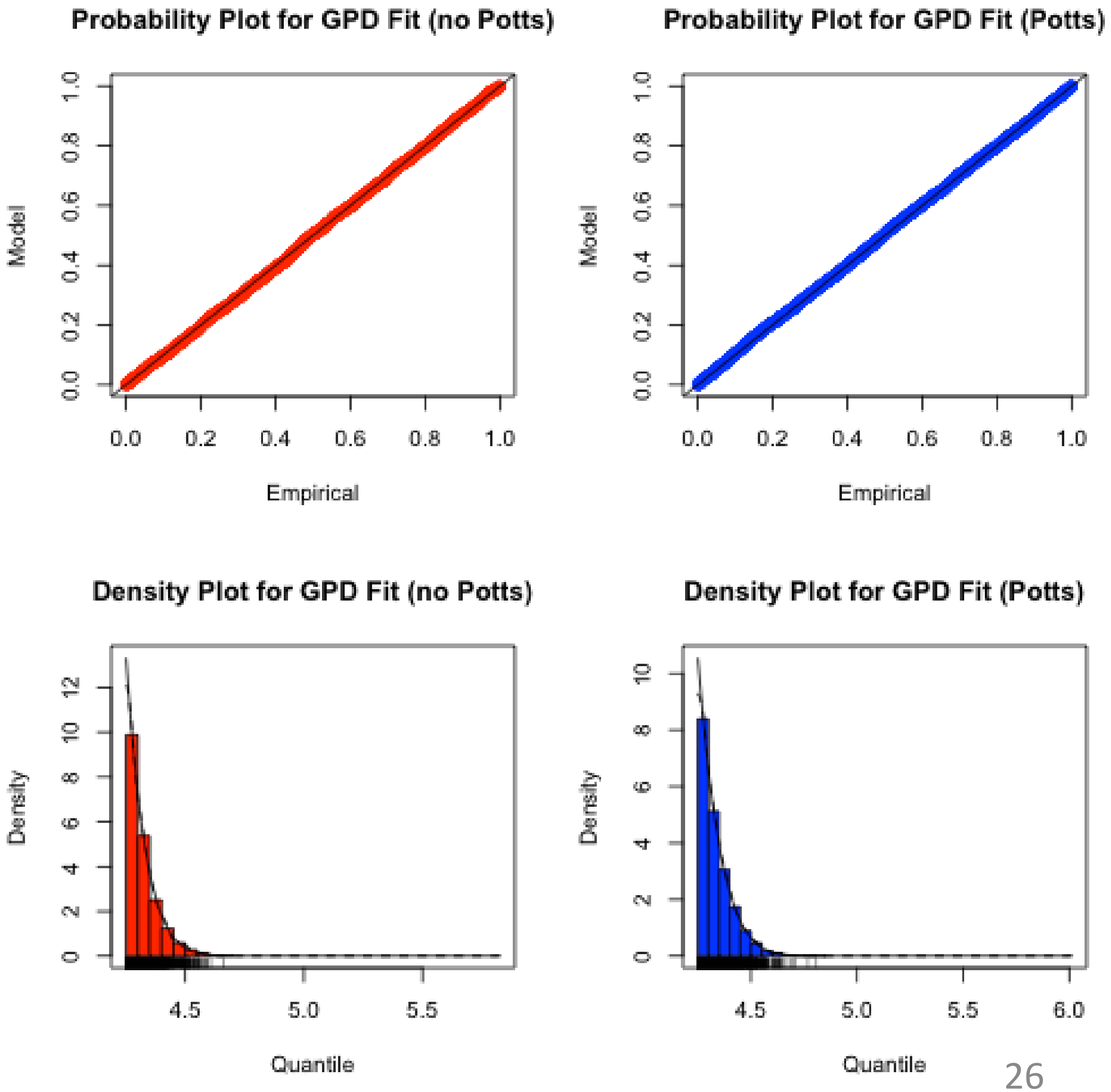
Extreme value theory allows for the EED “hot spots” observed in the teFFT simulation to be fit to the generalized Pareto distribution (GPD). The method used is known as peaks over threshold (POT). Data above a chosen threshold value is fit to the GPD using maximum-likelihood estimation.

J. Pickands: Ann. Stat., 1975, vol. 3, pp. 119-131.

Extreme Value Analysis: Peaks over Threshold

Fits for both types of interface are superficially similar. The Potts model data exhibits a larger scale parameter (0.095) compared to the flat interface data (0.075), indicating the Potts model data is more spread out.

	Potts Model	*No Potts*
scale	0.095	0.075
shape	-0.126	-0.095



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Summary

- The teFFT code was used to compute the thermal residual stresses in several test systems.
  - Industry standard TBC materials utilized.
  - Different microstructures tested. DREAM.3D has the capability to reproduce most observed microstructures.
  - Potts model applied layers near interfaces to induce undulating features.
- EED hot spots observed at interface defects, such as ridges.
- Extreme values in EED can be fit to the GPD using the POT approach, allowing for hot spots to be statistically analyzed.

Future Work

- Continue work on reproducing real TBC microstructures.
    - Inclusion of thermally grown oxide.
    - Reproduction of the true multi-phase nature of the bond coat.
    - Correct ratios of layer thickness to grain size.
- Test the scaling of the parallel teFFT on massively parallel systems.
    - The group currently has computational time available on the shared memory supercomputer Blacklight at the Pittsburgh Supercomputing Center, as well as access to the cluster at Oregon State University through NETL.
- Extend POT approach to allow for complete statistical analysis of the extreme values in EED.

Acknowledgments

- Dr. Ricardo Lebensohn of Los Alamos National Laboratory, for supplying a copy of the elastic FFT code.
- Ben Anglin, doctoral student in the Rollett group, for providing the thermoelastic FFT code, which is the modified version of Dr. Lebensohn’s code for computing thermoelastic eigenstrains.