Quantitative relationships between stress distributions, microstructure, and high strain rate performance of advanced ceramics: an interim report

Leigh L. Noble
MADN-MATH, USMA
West Point, NY 10996-1905
leigh.noble@usma.edu
http://www.math.usma.edu/people/Noble/

October 24, 2006[1]

Abstract

Ceramics often replace metal parts while providing improvements to a system. However, the exact relationship between characteristics of ceramic materials and mechanisms of failure is still being explored by the research community. This paper showcases current progress of an ongoing project concerning advanced ceramics under high strain rate and large strain conditions. The project places special emphasis on the effects of microstructure and the implications of highly variable internal stresses prior to cracking.

Numerical simulations created in OOF2, a program developed at NIST which uses object oriented finite elements to analyze real micrographs of microstructures, allow virtual experiments in two-dimensions. Progress towards visualizing effects of single crystal anisotropy on the stress between grains will be presented. Other simulations found in the literature highlight the fluctuation of internal stress states as material is stressed close to failure. Use of the mathematical concept of fractal dimension to characterize these stress states will be discussed.

1 Introduction

This paper highlights the research project currently being undertaken by the author. A paper introducing the project was presented at this same conference last year. [15]

On the smallest scale, all solids are composed of discrete molecules. Numerical simulations are a discretization of a continuous representation of the original discrete

[1]To be presented at the 14th Annual ARL/USMA Technical Symposium on November 1, 2006

system. This sounds somewhat circular and one might believe that molecular dynamics would be the most direct way to simulate behavior of a material. The enormous computing resources necessary to describe the shear numbers of atoms involved in simulating a bulk macroscopic material are coming into reach with each advance in computing power and molecular dynamics approaches hold great promise. Nevertheless, it seems the effects of grain level features on macroscopic behavior are lost in this approach. For this reason, other types of modeling continue to be used to probe mesoscale effects, and direct mathematical analysis is used to gain further insight into the governing relationships between microstructural features and macroscopic mechanical response.

1.1 Project Description

The aforementioned project is concerned with high compressive stress, high strain rate, and large strain conditions such as is likely in armor or ballistics applications of ceramics. The materials of focus are advanced ceramics such as boron carbide (B_4C), titanium diboride (TiB_2), silicon carbide (SiC), aluminum oxide (α-Al_2O_3), and aluminum oxynitride (AlON), a dual phase material containing aluminum oxide and aluminum nitride phases. Glass is generally excluded from consideration. Some of these materials have everyday uses, such as in cutting tools, mechanical seals, and insulating bodies.

The project has two main thrusts. The first is to determine the effects of microstructure on the response of advanced ceramics under high strain rate conditions. The microstructural features of particular interest to the project are crystallographic texture, misorientation, grain size, and grain geometry. The second is to expose and quantify any relationship between the distribution of internal stress in ceramic materials under high strain, large stress, and high strain rate conditions and the types or magnitudes of failure.

1.2 Focus and Organization of Paper

This paper reveals progress on two pieces of recent research related to this project. The first focus is to create numerical simulations of the effects of stress on real microstructures exhibiting texture. The second focus is to determine if fractal dimension can be used to characterize the temporal and spatial fluctuations in the stresses prior to cracking. These two pieces are aligned with the main thrusts of the project defined in the previous paragraph. This research is ongoing and only basic information is

ready for presentation here. A paper with final results is expected to be published at a later date.

Sections 2.1 and 3.1 provide background for the discussions in those sections. Section 2.2 covers the current progress in using numerical simulation software to show stress across grain boundaries in real microstructures. Section 3.2 contains a discussion of the possibility of relating fractal dimension to the distribution of internal stress states. Sections 4 and 5 conclude the paper with a short summary and acknowledgements.

2 Effects of Anisotropy

Ceramics are manufactured through sintering, a process by which powders are compressed and then heated to encourage strong interparticle bonding. Other processing may involve hot isostatic pressing (frequently abbreviated "HIP"), microwave sintering, and dynamic compaction [18]. After sintering, it is possible for the polycrystalline form to be nearly isotropic; however, the manufacturing process can impart *texture* or preferred orientation of the crystallites in the bulk solid.

2.1 Background

Texture is frequently described using the orientation distribution function

$$w(\psi, \theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} W_{\ell mn} Z_{\ell mn}(\cos\theta) e^{-im\psi} e^{-in\phi}$$

after Roe's notation [17]. In common use for metal materials, this orientation distribution function may be used to describe textures in ceramic materials as well. The triple (ψ, θ, ϕ) are Euler angles indicating a rotation with respect to a fixed reference orientation; $W_{\ell mn}$ are known as the *texture coefficients*, and $Z_{\ell mn}$ are Jacobi polynomials. The influence of the coefficients dwindles as ℓ increases[2], and under specific crystal and sample symmetries many of the $W_{\ell mn}$ are zero or linearly dependent.

In practice, various properties such as strength or plasticity are correlated with specific coefficients in certain metals. By considering the elasticity tensor $\mathbb{C}$ to be a function of the orientation distribution function w, i.e. $\mathbb{C} = \mathbb{C}(w)$, Man worked out the relationship between texture coefficients and elastic constants for metals under certain underlying conditions [10, 11, 12].

[2] In computer programs, w is often truncated at $\ell = 22$.

Single crystals of ceramic materials can be highly anisotropic. Titanium diboride forms hexagonal crystals, boron carbide forms rhombohedral crystals, and silicon carbide forms cubic (β-SiC), or hexagonal or rhombohedral (α-SiC) crystals [14, 18]. The crystal symmetry must be taken into account for proper measurement of single crystal elastic constants. Numerical and analytical models should take into consideration symmetry of the crystals as well as the texture of the bulk solid.

A generalization of Hooke's law is frequently written $\boldsymbol{\sigma} = \mathbb{C}[\boldsymbol{E}]$ where $\boldsymbol{\sigma}$ is the stress, $\boldsymbol{E}$ is the strain, and $\mathbb{C}$ is the fourth order tensor with entries denoted $C_{ijk\ell}$ known as *elasticity constants*. Hooke's law is a linear relationship valid only at small strains. In studying the response of ceramics under the high strain conditions mentioned above, the linear theory may no longer apply. The non-linear stress-strain relationship $\boldsymbol{\sigma} = \mathbb{C}[\boldsymbol{E}] + \mathbb{D}[\boldsymbol{E}]$, where $\mathbb{D}$ is a sixth order tensor, may be a better description of the stress-strain relationship in the cases of interest to this project, but such a relationship is difficult to use in practice. In any event, if $\mathbb{C}$ is affected by w, the stress will be too. The orientation distribution function w may be a powerful analytical tool to characterize the texture of ceramics and predict properties of specific samples. A future topic of experimental research could be to determine whether mechanical properties can be correlated to specific texture coefficients for ceramics as for metals. The program `OOF2`, discussed next, is a step towards visualizing the effects of crystallographic orientation on the stress between grains.

2.2 Visualization with `OOF2`

`OOF2` is an object oriented implementation of the finite element method designed to solve heat and force balance equations (and some others) on two-dimensional images of real microstructures. The program was produced by the Center for Theoretical and Computational Materials Science at the National Institute of Standards and Technology. It is freely available for download and can be found on their homepage [2]. The program can be expanded to include additional fields, properties, or equations as the user requires. In addition, the mesh geometries it creates can be input into the commercial finite element package ABAQUS.

The `OOF2` program is specially designed to run simulations on real microstructures. Figure 1 shows a graphical solution of the heat equation

$$\begin{cases} \nabla \cdot J &= -\frac{\partial U}{\partial t} \\ \frac{\partial U}{\partial n} &= 5 \qquad \text{on left and right boundaries} \\ U &= 5 \qquad \text{on top boundary} \end{cases}$$

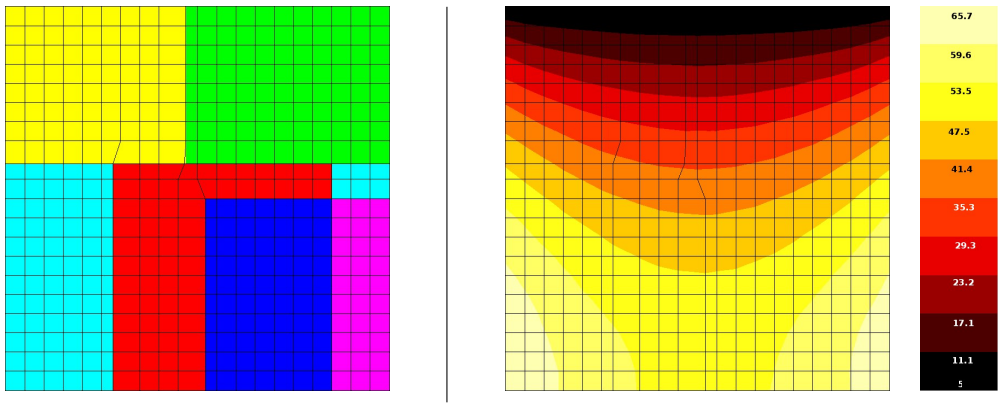

Figure 1: Left: Initial simulated microstructure and mesh. Right: Temperature.

which can be created by a skillful operator in just a few minutes. The domain is a simulated micrograph and version 2.0.1 of `OOF2` was used.

Some advantages of using a program such as `OOF2` are:

- A prepared package reduces the need to implement meshing and finite element analysis from scratch;
- Creating and refining meshes can be done with a few mouse clicks;
- `OOF2` is specifically designed for use on actual micrographs;
- Extending the functionality can be done in `C++` or the easily readable `Python`.

In the future, `OOF2` developers hope to include direct support for plasticity, time dependence of fields and properties, and parallel execution.[3]

By the 1960s basic equations of thermo-anisotropic elasticity were well known and anisotropic thermal contractions had been proposed as the driving mechanism for changes in internal stresses leading to fracture of brittle ceramics [19, p. 218] [3, p. 506]. For anisotropic materials under the large strain, high strain rate conditions being studied, it would be wise not to neglect thermal effects. The thermo-anisotropic

[3] As seen at `http://www.ctcms.nist.gov/oof/oof2/index.html`, accessed October 19, 2006.

elasticity equations[4] are:

$$
\begin{aligned}
\sigma_{ij} &= \mathbb{C}_{ijk\ell} u_{k,\ell} - \beta_{ij} T && \text{stress-strain law} \\
\sigma_{ij,j} &= 0 && \text{equilibrium} \\
h_i &= -\kappa_{ij} T_{,j} && \text{heat conduction} \\
h_{i,i} &= 0 && \text{balance of energy}
\end{aligned}
$$

where β_{ij} are thermal moduli, κ_{ij} are heat conduction coefficients, and $\mathbb{C}_{ijk\ell}$ are the elastic constants. T. C.-T. Ting uses Stroh's formalism to give a solution using for the two-dimensional case in [3].

Solving these equations numerically with `OOF2` should produce a way to view the stress between grain boundaries. The following steps are underway:

1. Solve using simulated data on a simulated micrograph,
2. Solve using simulated data on a real micrograph, and
3. Solve using real data on a real micrograph.

Currently, step 1 is in progress and steps 2 and 3 are in the planning stages.[5] Results from step 1 would clearly illustrate the effects of grain-level anisotropies on the internal stress state of a ceramic material; the last two steps would illustrate the same concept on an actual sample.

Besides producing a nice illustration showing the effects of single crystal anisotropy on stress between grains, it might be possible to extend `OOF2` to include texture effects. Furthermore, the numerical data from `OOF2` output could possibly be used to input texture related data into a more sophisticated model for high velocity impacts such as the Johnson-Holmquist-Beissel (JHB) model.[6] (For more information on the JHB and related models, references [7] and [9] are recommended.) Testing the concept of using

[4] All indices are from 1 to 3. A comma followed by an index indicates a spatial derivative and repeated indices indicate summation. For example, $\sigma_{ij,j} = 0$ means

$$
\begin{cases}
\partial\sigma_{11}/\partial x_1 + \partial\sigma_{12}/\partial x_2 + \partial\sigma_{13}/\partial x_3 &= 0 \\
\partial\sigma_{21}/\partial x_1 + \partial\sigma_{22}/\partial x_2 + \partial\sigma_{23}/\partial x_3 &= 0 \\
\partial\sigma_{31}/\partial x_1 + \partial\sigma_{32}/\partial x_2 + \partial\sigma_{33}/\partial x_3 &= 0.
\end{cases}
$$

[5] In these steps, the term "real" means data obtained through physical experiments. Micrographs are relatively easy to obtain; however, the related elastic constants, thermal moduli, and crystallographic orientations of grains are more difficult. Plans to obtain that information are underway now.

[6] This suggestion came from Jeff Swab for during a discussion about the `OOF2` package and this project.

OOF2 to solve the thermo-anisotropic elasticity equations and including texture effects must be completed before determining the best way to incorporate the information learned into other models.

3 Stress Fluctuations

In the previous symposium, results from three papers were presented [15] to support the idea that internal stress distributions have important consequences on the integrity of material close to failure. The papers all used different types of numerical simulations to model fracture but in each paper unexpected or unusual fluctuations of internal stress states were noted. A quick summary of the papers is presented again here for completeness.

3.1 Background

In the 2004 paper by X. H. Zhang, *et al.* [22], a heterogeneous media in tension was simulated using a two-dimensional network of six bars hinged at each point. When a bar broke in this model, the stress was redistributed throughout the network, similar to a network of fuses carrying current. The differing yield stresses and orientations of the bars modeled strength at the mesoscopic scale. Zhang's simulation showed three stages leading to damage:

1. Formation of small cracks (microcracks) while macroscopically the material was still within the linear stress-strain range.

2. An increase in damage while high stresses shifted rapidly from one physical location to another in the material.

3. The appearance of large cracks with the crack tip becoming the location of largest stress concentration.

The sample ruptured catastrophically prior to the maximum stress predicted in a traditional mean field approximation model. A conclusion was drawn that a major difficulty in predicting rupture was the coupling between stress fluctuations mentioned in stage 2 above and sample specific heterogeneity.

In a paper published in 2005, D. Zhang, *et al.* [21] created a computational model designed to test the effects of various microstructural elements on the deformation of α-6H silicon carbide (SiC) under uniaxial strain compression past the Hugoniot

elastic limit (modeling high confinement during the steady-state portion of shock compression). Single crystal slip was allowed, but fracture was not. Data analysis presented by D. Zhang, *et al.* found that the mean and standard deviation of both the longitudinal and lateral stresses increased as applied compression increased. Since standard deviation is a measure of heterogeneity, this result is interpreted to mean that the stress states in the material become increasingly complicated as the material is stressed close to failure.

In another 2005 paper, Tasdemirci and Hall [20] performed experiments on multilayered material (aluminum oxide face plate, low modulus interlayer, glass/epoxy backing plate) using a Split Hopkinson Pressure Bar. Their data supported the idea that severe stress heterogeneity has more serious consequences on the integrity of the material than one would conclude from looking at maximum stress alone.

These papers give a glimpse into what could be a useful tool to predict rupture or severe cracking: the level of heterogeneity of internal stress on the mesoscopic scale. All three authors reported that the fluctuations in internal stress states significantly affected integrity of the material. Mean field approximations do not seem adequate to predict cracking; new or revised theories need development. The coupling between the stress states and the heterogeneity of each specific sample is not clearly understood. Understanding these stress fluctuations may lead to a better understanding of cracking.

3.2 Fractal Dimension

This author proposes to use fractal dimension to characterize stress fluctuation and perhaps to define a threshold dimension which would indicate a crack is imminent. There are many ways to define dimension leading to possibly fractional values for dimension [4, p. xx] [13]. The most basic definition of fractal dimension is the *box-counting* or *self-similarity* dimension.

Definition 3.1 ***self-similarity dimension***
Given a self-similar object of N parts scaled by the ratio r from the whole, its fractal dimension is

$$D = \frac{\log N}{\log (1/r)}.$$

$\triangle$ [1, p. 28]

When different subsets of the object exhibit different dimensions the object is considered to be *multifractal* and leads naturally to the study of the singularity spectrum

of the multifractal dimension [4, Chpt 17].

The objects to study in this project are the stresses at each point for fixed times as the material is deformed. This is in contrast to the work of Herrmann [6], who noted the multifractality with respect to the appearance of local strain, and others such as Hansen and Roux [5] who used multifractals to describe the geometrical appearance of cracking.

Two cautionary notes are appropriate here. The author is not currently aware of any way to measure these stress heterogeneities *in situ* during a high strain rate event so only numerical simulations are available to corroborate advances in theory. This should not be interpreted to mean that pursuit of this idea will be meritless. Certainly understanding the reason and mechanism of cracking are the important concepts; new physical measurement techniques can be developed in the future. If this method does not lend itself to a better explanation of behavior, the difficulties associated with physical experimental evidence of fractal dimension of internal stress distributions during high strain rate events will be irrelevant. A second cause for caution is that it is possible that the stress heterogeneity seen in the simulations could be the result of scattering in the numerical calculation itself due to computational limitations [16]. If this is the case, it will be discovered quite early in the development of the fractal dimension framework. Without knowing more details of the implementations of the numerical simulations outlined at the beginning of Section 3, this author can only speculate when saying that the same behavior in three different models suggests otherwise.

To advance the idea of using fractal dimension to characterize stress fluctuations prior to cracking, the specific definition of dimension to be employed in the theory should be determined. A method to calculate the fractal dimension of a stress state during the simulation of a high strain rate or high stress event needs to be tested. Not all definitions of dimension lend themselves to numerical calculation; it would be advantageous to use one that does, but this is not required for the theory. Uses of the multifractal spectrum concept need to be learned and appropriate applications suggested with respect to this project. Developments involving the concept of multifractals to characterize the stress distribution of a ceramic under high strain rate conditions will be reported as they are achieved.

4 Summary

Investigation of fracture of armor ceramics under high strain rate, high stress conditions proves to be intriguing. The problem outlined in this overall project is not trivial or easy as evidenced by the recent Oak Ridge National Laboratory announcement of 1.5 million processing hours awarded to researchers hoping to "gain insight into how materials fracture, which despite decades of study remains a fundamental problem of science and engineering" [8].

A more complete understanding of cracking under the conditions in this project will ultimately call for investigation of other effects such as the relationship of slip to fracture and the effects of grain size and shape on material response. Making progress on the two thrusts outlined here:

- using `OOF2` to solve the thermo-anisotropic elasticity equations, and
- calculating the fractal dimension of a stress distribution prior to cracking,

will be a useful advance. Success in these endeavors places the theory on the path to utilizing texture data in more sophisticated finite element codes and characterizing multifractal stress modes leading to failure. This is a step towards a more complete picture of this "fundamental problem."

5 Acknowledgements

This research was performed while the author held a National Research Council postdoctoral fellowship at the United States Military Academy (USMA) in West Point, NY and the Army Research Lab (ARL) in Aberdeen, MD. This work would not have been possible without the input and direction provided by ARL advisers James W. McCauley and Thomas W. Wright. Many thanks are extended to the two of them. The author also appreciates the helpful conversations with Jeff Swab of ARL and the encouragement of Amy H Erickson of USMA.

References

[1] Michael F. Barnsley, Robert L. Devaney, Benoit B. Mandelbrot, Heinz-Otto Peitgen, Dietmar Saupe, and Richard F. Voss. *The Science of Fractal Images*. Springer-Verlag, New York, 1988. ISBN 0-387-96608-0.

[2] Center for Theoretical and Computational Materials Science at the National Institute of Standards and Technology. http://www.ctcms.nist.gov/oof/. Last accessed October 19, 2006.

[3] Thomas Chi-Tsai Ting. *Anisotropic Elasticity: theory and applications*, volume 45 of *Oxford Engineering Series*. Oxford University Press, 1996. ISBN 0-19-507447-5.

[4] Kenneth Falconer. *Fractal Geometry: Mathematical Foundations and Applications*. John Wiley & Sons Ltd., 1990. ISBN 0-471-92287-0.

[5] A. Hansen and S. Roux. Statistics toolbox for damage and fracture. In Dusan Krajcinovic and Jan Van Mier, editors, *Damage and Fracture of Disordered Materials*, volume 410 of *International Centre for Mechanical Sciences Courses and Lectures*, chapter 2, pages 17–101. Springer-Verlag Wien New York, 2000.

[6] H[ans] J. Herrmann. Fracture patterns and scaling laws. *Physica A*, 163:359–372, 1990.

[7] Timothy J. Holmquist and Gordon R. Johnson. Characterization and evaluation of silicon carbide for high-velocity impact. *Journal of Applied Physics*, 97, 2005. DOI: 10.1063/1.1881798.

[8] HPCWire. Posted at http://www.hpcwire.com/hpc/586343.html the week of March 10, 2006 and mirrored at http://www.csm.ornl.gov/PR/PR2006/hpc-03-10-06.html. Last accessed October 19, 2006.

[9] Gordon R. Johnson, Timothy J. Holmquist, and Stephen R. Beissel. Response of aluminum nitride (including a phase change) to large strains, high strain rates, and high pressures. *Journal of Applied Physics*, 94(3):1639–1646, August 2003.

[10] Chi-Sing Man. Effects of texture on plastic anisotropy in sheet metals. In Robert E. Green, Jr., editor, *Nondestructive Characterization of Material VIII*, pages 751–756. Plenum Press, 1998.

[11] Chi-Sing Man. On the constitutive equations of some weakly-textured materials. *Arch. Rational Mech. Anal.*, 143:77–103, 1998.

[12] Chi-Sing Man. Effects of crystallographic texture on the acoustoelastic coefficients of polycrystals. *Nondestructive Testing and Evaluation*, 15(3–4):191–214, 1999.

[13] Yuri I. Manin. The notion of dimension in geometry and algebra. *Bulletin of the American Mathematical Society (N.S.)*, 43(2):139–161, 2006.

[14] Ronald G. Munro. Material properties of titanium diboride. *Journal of Research of the National Institute of Standards and Technology*, 105(5):709–720, 2000.

[15] Leigh L. Noble. Quantitative relationships between stress distributions, microstructure, and high strain rate performance of advanced ceramics: a preliminary report. In *Proceedings of 13th Annual ARL-USMA Technical Symposium*, 2005.

[16] Pat Quillen. Personal communication, July 2006. Currently at The MathWorks.

[17] Ryong-Joon Roe. Description of crystalline orientation in polycrystalline materials. III. General solutions to pole figure inversion. *Journal of Applied Physics*, 36(6):2024–2031, 1965.

[18] R.E. Smallman and R.J. Bishop. *Modern Physical Metallurgy and Materials Engineering*. Butterworth-Heinemann, Woburn, MA, sixth edition, 1999.

[19] R. J. Stokes. Microscopic aspects of fracture in ceramics. In H[arold] Liebowitz, editor, *Fracture of Nonmetals and Composites*, volume VII of *Fracture: An Advanced Treatise*, chapter 4, pages 157–241. Academic Press, New York, 1972.

[20] A. Tasdemirci and I. W. Hall. Experimental and modeling studies of stress wave propagation in multilayer composite materials: Low modulus interlayer effects. *Journal of Composite Materials*, 39(11):981–1005, 2005.

[21] D. Zhang, M. S. Wu, and R. Feng. Micromechanical investigation of heterogeneous microplasticity in ceramics deformed under high confining stresses. *Mechanics of Materials*, 37:95–112, 2005.

[22] X. H. Zhang, F. Rong, Z. K. Jia, F. J. Ke, M. F. Xia, and Y. L. Bai. Coupling effects of heterogeneity and stress fluctuation on rupture. *Theoretical and Applied Fracture Mechanics*, 41:381–389, 2004.