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

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October 15, 2005[1]

Abstract

Ceramics have become useful and productive in engineering applications, often replacing metal parts while providing improvements to the system. However, the relationship between characteristics of ceramic materials and measured properties is still being explored by the scientific community. This study focuses on ceramics under high compressive stress, high pressure, large strain, and high strain rate, particularly the effects of microstructure and the implications of irregular stress distributions. Preliminary studies on microstructure and stress conditions in ceramics are presented.

Much mathematical and engineering literature has been devoted to the influence of microstructure in metals. One aim of this study is to clarify the mathematical dependencies of microstructure such as preferred grain orientation, misorientation, and grain geometry in constitutive equations governing the behavior of ceramics. In addition, inspired by literature showing unexpected stress distributions in simulations of ceramics under high strain rate conditions, relationships between the distribution of stress in a ceramic material and the material's behavior are explored.

1 Introduction

This paper serves as an introduction to the research currently being undertaken by the author. There are two main thrusts to the project. The first is to determine the effects of microstructure on the response of ceramics under high strain rate conditions. The microstructural features of particular interest in this project are crystallographic texture, misorientation, grain size, and grain geometry. The second is to expose

[1]To be presented at the 13th Annual ARL/USMA Technical Symposium on November 2, 2005

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 in ceramics. As this project is in the early stage, this paper gives a qualitative summary of background evidence and ongoing work.

On the smallest scale, all solids are composed of discrete molecules. When numerical simulations are performed, we are looking at a discretization of a continuous representation of the original discrete system. This sounds somewhat circular. Molecular dynamics would be the most direct way to simulate crack growth in a material but even with modern computers it is still prohibitively expensive to model the sheer numbers of atoms in a bulk macroscopic material. Hence other forms of analysis continue to be used. It is for this reason that we investigate the affects of microstructure and stress distributions on ceramic behavior. Not only do we hope to gain further insight into the role of these characteristics but we may find ways to predict failure with greater accuracy.

This work is concerned with high compressive stress, high strain rate, and high strain conditions such as is likely in armor or ballistics applications. The focus will be on materials 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. Some of these materials have everyday uses, such as in cutting tools, mechanical seals, and insulating bodies. Glass is generally excluded from the discussion to follow.

2 Microstructure

Ceramics differ from metals in that the bonds between atoms are either ionic or covalent, or a mixture [13], rather than metallic, but like metals, they are not organic compounds. 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, microwave sintering, and dynamic compaction. 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. The crystal symmetry must be taken into account for proper measurement of single crystal elastic constants. After sintering, it is possible for the polycrystalline form to be nearly isotropic; however, the manufacturing process often imparts texture or preferred orientation of the crystallites in the bulk solid. Models must take into

consideration symmetry of the crystals as well as the texture of the bulk solid. [10, 13]

In metals, texture is frequently described using the orientation distribution function

$$w(\psi, \theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} W_{\ell mn} Z_{\ell mn}(\cos\theta) e^{-im\psi} e^{-in\phi} \tag{1}$$

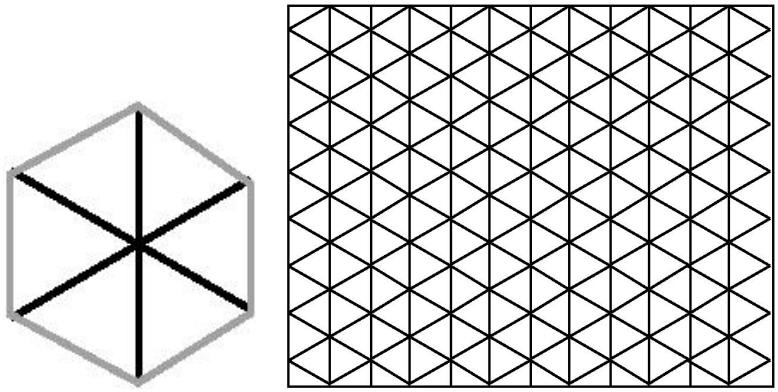
after Roe's notation [12]. This orientation distribution function can be used to describe textures in ceramic materials. The (ψ, θ, ϕ) are Euler angles indicating a rotation with respect to a fixed reference orientation; $W_{\ell mn}$ are known as the *texture coefficients*, and $Z_{\ell mn}$ are Jacobi polynomials. The influence of the coefficients dwindles as ℓ increases, and under specific crystal and sample symmetries many of the $W_{\ell mn}$ are zero or linearly dependent. In computer programs, w is often truncated at $\ell = 22$. In practice, it has been found that for metals certain properties such as strength or plasticity are correlated with specific coefficients [7]. Similar relationships should be checked in ceramics. The orientation distribution function could be a powerful analysis tool to characterize the texture of ceramics and predict properties of specific samples.

Misorientation is a measure of the relative differences in orientations of adjacent grains. Sometimes this is described as a "grain boundary texture" [4, p. 97]. As mentioned at the beginning of this section, ceramics are polycrystalline like metals and so the same methods used to analyze misorientation in metals should be applicable to ceramics under the same assumptions. As of the writing of this report, this author has not yet researched the effects of misorientation.

Just as in metals, grain size and shape will affect the response and characteristics of ceramics. For example, in TiB_2, grain size was shown to affect fracture toughness [10, p. 713]. Here we speak of a grain as being composed of crystallites having a single orientation with its border being the spatial locations where it touches crystallites having other orientations. Two extreme shapes would be equiaxed (or spherical) grains and elongated (or flattened) grains. Generally the effects of grain geometry are difficult to separate from the effects of texture. Average grain diameter of metals can be estimated through ultrasonic attention measurements [3]. Another way to quantify grain shape is through the mean linear intercept [15]. Further study of grain morphology will be required.

As explained, we should be able to proceed the same way in describing and analyzing microstructure as has been done with metals. A large body of work exists on weakly textured orthorhombic aggregates of cubic crystallites (e.g. aluminum sheets), but typical sample symmetries imposed by the manufacturing processes for ceram-

Figure 1: Diagrams of 6 bars hinged together (left) and network of bars (right)



ics will need to be determined through the literature or other means. The reader is cautioned that size effects may be different between ceramics and metals. For example, where one type of texture generally dominates or predicts a certain response in metals, one must be careful to reconsider the analysis in order to be certain that it is not based on assumptions or empirical evidence not applicable to ceramics. Otherwise, one may find that particular microstructure characterization does not predict accurately the behavior of a ceramic material.

3 Stress Distribution

In the recent paper by X. H. Zhang, *et al.* [17], a heterogeneous media in tension was simulated using a two-dimensional network of 6 bars hinged at each point (see Figure 1). Each bar was assigned the same elastic modulus but an individual yield point. Yield points followed a Weibull distribution but were spatially uncorrelated. Every bar deformed elastically until the local stress reached its individual yield point, at which time the bar would break. When a bar broke in this model, the stress was redistributed throughout the network, similar to a network of fuses carrying current. (See [2, pp. 43–55] for a detailed description of this type of model.) The differing yield stresses and orientations of the bars modeled strength at the mesoscopic scale (between the macro and atomic scales). 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.

This type of model, although seemingly simple, is surprisingly useful. The philosophy behind the model is to strip out all unnecessary features of the material being modeled and leave only the features primary to the behavior being studied. It is thought that materials fracture because the stress is higher at the point where it fractures or the material is relatively weaker at that location. [2] This network model satisfies these two possibilities and assumes little else about the material. Lest one not believe the conclusions drawn from this network model, additional models are discussed next.

In a paper published in 2005, D. Zhang, *et al.* [16] created a computational model more elaborate than X. H. Zhang's 2004 network model. The simulation in [16] was 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). Hexagonal grains were simulated in an isotropic solid; 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 increase as applied compression increases. Standard deviation is a measure of heterogeneity. Like the simpler example, 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 [14] 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.

All of these papers give a glimpse into what could be a useful tool to predict rupture or severe cracking: the level of heterogeneity of stress on the mesoscopic scale.

4 Ongoing Work

Many authors seem to desire to find a "magic number" that will indicate whether a fracture or crack will occur or whether a material will fail at a specific stress or strain level. This author has doubts as to whether it is reasonable to quantify the response of a material in a single parameter and then try to use that single parameter to predict fracture or failure. Certainly it seems unreasonable to expect a single or averaged quantity to give an indication as to the location of a crack. Location information could ultimately prove more useful than whether or not a crack occurs. Perhaps it would be more fruitful to try to use statistics to show where fracture or failure is likely to occur. However, predicting a crack location may be further than we are ready to go in this project. The three papers ([17, 16, 14]) referred to in Section 3 may be narrowing in on a better idea— one of using some measure of stress heterogeneity to predict cracking or failure. To this end it may be possible to use the theory of multifractal formalism. This formalism has been applied to many problems, including turbulence, but this author has not yet studied the method.

An interesting result of the work by D. Zhang, *et al.* [16] involving simulation of single crystal slip in ceramics is that the specific slip systems activated affected the shape of the stress distribution. When basal and prismatic slip systems were activated, the resulting stress distribution became bi-modal. The relationship of slip to local stress and fracture will need scrutiny.

Further review of the literature concerning ceramics and microstructure needs to be done. In particular, analysis of the dependence of specific characteristics on certain texture coefficients should be determined. The affects of grain size and shape on material response still need to be mastered. This research should lead to further insight on the nature of damage in ceramics and the response of ceramics under high strain and high strain rate conditions.

5 Related Future Topics

The plans in Section 4 indicate much work still to be done on this project. Yet, several related questions have arisen. This section outlines potential topics which may not be covered under the immediate project, but might provide insight into the behavior of ceramics.

Due to their manufacturing process, ceramics are composed of many more voids than are typical of metals. These voids have a significant effect on the response of

the ceramics. In addition, large numbers of microcracks can reach a critical level and lead to failure or develop into cracks which adversely affect the structural integrity of the sample. Voids and microcracks are two additional microstructural features which may be studied at a later date.

Biologically useful ceramics are manufactured to strict specifications with expectations of high reliability under extreme conditions. Some such ceramics are Procera brand Al_2O_3, Ti-TiB [2], B_4C-Al_2O_3, and NI-TL $Ca_3(PO_4)_2$ [3]. In order to facilitate grafting between artificial and natural bone, the ceramics used in bone replacement applications are porous. These materials are purposely made with voids in an attempt to mimic natural bone structure so living bone will grow into them. It is interesting to this author to learn that these materials have been grown most successfully in space. A future project would include testing the models developed in this project against these biological materials.

Lastly, some ceramics, such as ceramic matrix composites, have microstructures which are not clearly classified with the texture function in Equation (1). The formation of whiskers[4] inside the bulk matrix can strongly affect the response of the ceramic. A method to characterize textures which includes whiskers and similar phenomenon should be considered.

6 Acknowledgments

This research was performed while the author held a National Research Council Research Associateship Award at the United States Military Academy in West Point, NY and the Army Research Lab in Aberdeen, MD. Discussions with the team of James W. McCauley and Thomas W. Wright of the US Army Research Laboratory, along with resources they provided, made this work possible. This author also appreciates the inspiration and assistance of Rachelle DeCoste, a colleague at USMA-West Point who read every version of this report.

[2]See `http://www.mines.edu/research/ccacs/Porous_Ceramics/Porous_Ceramics.html`

[3]See `http://microgravity.grc.nasa.gov/fcarchive/combustion/papers/Schowengerdt/Combustion_Synthesis_of.htm`

[4]A nice photo of whiskers in TiB can be seen in Figure 2 of [11] which, at the date of this report, can also be seen online at `http://www.tms.org/pubs/journals/JOM/0405/Chandran-0405.html`

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