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by John D. Clayton, R. Brian Leavy, and Reuben H. Kraft

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DYNAMIC COMPRESSIBILITY, SHEAR STRENGTH, AND FRACTURE BEHAVIOR OF CERAMIC MICROSTRUCTURES PREDICTED FROM MESOSCALE MODELS

John D. Clayton¹, R. Brian Leavy¹, and Reuben H. Kraft¹

¹RDRL-WMP-B, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21005-5066

Abstract. Fundamental understanding of dynamic behavior of polycrystalline ceramics is advanced through constitutive theory development and computational modeling. At the mesoscale, microstructures of silicon carbide grains (hexagonal crystal structure) or aluminum oxynitride grains (cubic crystal structure) are subjected to compression or shear at high rates with varying confining pressure. Each grain is resolved by numerous three-dimensional finite elements, and behavior of each grain is modeled using nonlinear anisotropic elasticity. Cohesive fracture models and post-fracture contact are included. Normal and Weibull failure statistics from many simulations are collected and analyzed. Results demonstrate effects of load directionality, confinement, dilatation, elastic anisotropy and elastic nonlinearity, and grain boundary fracture properties on macroscopic (average) failure stresses for loading conditions in the ballistic regime. Predictions demonstrate reasonable agreement with data from macroscopic plate impact, unconfined compression, and flexure experiments.

Keywords: mesoscale, ceramics, silicon carbide, aluminum oxynitride, shock compression, fracture.

PACS: 62.20.-x, 62.20.D-, 62.20.-mj, 81.05.Je.

INTRODUCTION

Dynamic deformation and failure behaviors of high-strength ceramics are of interest for military and industrial applications. Properties of importance in the ballistic loading regime include hardness, elastic stiffness, fracture toughness, unconfined compressive strength, dynamic shear strength, and failure probabilities [1-6]. The present work investigates two ceramic materials: silicon carbide (SiC) and aluminum oxynitride (AlON). Mesoscale models are used, wherein each grain in a polycrystalline aggregate is resolved explicitly in a numerical simulation.

This paper is organized as follows. First, models for single crystals and interfacial fracture are listed. Next, three-dimensional microstructures depicted using finite elements are described. Results of simulations considering uniaxial strain

compression, uniaxial stress compression, and shear boundary conditions are reported. Finally, statistics of dynamic failure are analyzed.

THEORY

Essential aspects of the constitutive theory are given here; a comprehensive description will be published later [7]. Consider hyperelastic behavior of single crystals [8-10] within a given polycrystal. Spatial and material coordinates are related by

$$x^a = x^a(X^A, t), \quad (1)$$

where t denotes time. The deformation gradient is

$$F_{\cdot A}^a = \partial x^a / \partial X^A. \quad (2)$$

The symmetric Lagrangian elastic strain is

$$E_{AB} = \frac{1}{2}(F_{\cdot A}^a F_{aB} - G_{AB}), \quad (3)$$

with G_{AB} the covariant referential metric tensor.

Assuming isentropic behavior, internal energy density per unit reference volume U is, to third order in strain,

$$U = \frac{1}{2} C^{ABCD} E_{AB} E_{CD} + \frac{1}{6} C^{ABCDEF} E_{AB} E_{CD} E_{EF} \quad (4)$$

In Voigt's notation, second- and third-order elastic constants $C^{ABCD} \leftrightarrow C_{\alpha\beta}$ and $C^{ABCDEF} \leftrightarrow C_{\alpha\beta\chi}$.

The first Piola-Kirchhoff stress is

$$\begin{aligned} P^{aA} &= J F^{-1A} \sigma^{ab} = \partial U / \partial F_{aA} \\ &= F_{.B}^a (C^{ABCD} E_{CD} + \frac{1}{2} C^{ABCDEF} E_{CD} E_{EF}), \end{aligned} \quad (5)$$

where $J = \rho_0 / \rho$ is the Jacobian determinant of (2) and σ^{ab} is the Cauchy stress. In the absence of measurements of third-order elastic constants, pressure derivatives of second-order coefficients provide the following approximation [11, 12]:

$$\begin{aligned} C^{ABCDEF} &\approx -\frac{B}{3} \left(\frac{d}{dp} C^{ABCD} G^{EF} + \frac{d}{dp} C^{CDEF} G^{AB} \right. \\ &\quad \left. + \frac{d}{dp} C^{EFAB} G^{CD} \right), \end{aligned} \quad (6)$$

where $p = -\frac{1}{3} \sigma_{.a}^a$ is the Cauchy pressure and

$$B = -J(dp/dJ) = \rho(dp/d\rho) \quad (7)$$

is the bulk modulus, in (6) measured at $J = 1$. Properties for SiC and AlON single crystals are listed in Table 1 [11-15].

TABLE 1. Elastic properties for SiC and AlON crystals.

Property ^a	Value (SiC) ^b	Value (AlON) ^c
C_{11}	5.01	3.01
C_{12}	1.12	1.55
C_{44}	1.61	1.74
C_{13}	0.52	($=C_{12}$)
C_{33}	5.49	($=C_{11}$)
C_{111}	-8.44	-10.39
C_{112}	-8.73	-7.13
C_{113}	-8.73	-7.13
C_{123}	-8.88	-5.50
C_{133}	-8.73	-7.13
C_{144}	0.15	-0.81
C_{155}	0.15	-0.81
C_{222}	-8.44	-10.39
C_{333}	-8.44	-10.39
C_{344}	0.15	-0.81
Bulk modulus B	2.22	2.04
Shear modulus G	1.94	1.34
Poisson's ratio ν	0.16	0.23
Density ρ_0 [g/cm ³]	3.227	3.714

^aElastic constants $C_{\alpha\beta}$ and $C_{\alpha\beta\chi}$ in units of Mbar;

Eq. (6) used for $C_{\alpha\beta\chi}$.

^bReferences [11, 13]. ^cReferences [12, 14, 15].

A cohesive zone model addresses intergranular fracture, i.e., stress-induced separation between grains in a given polycrystal [14, 16-20]. Each grain in a polycrystal is treated as a distinct solid body interacting via contact with surrounding grains [21]. Prior to attainment of critical traction t_c , contact between grains is rigid (i.e., perfect bonding). When stresses are sufficient such that the critical traction is achieved at a given interface, separation ensues, with traction held at the critical level until complete separation occurs beyond distance δ_c . Analogous relationships and identical material properties are used for mode I (normal) and mode II (tangential) fracture. Bulk elastic and surface properties are related by [17, 20]

$$t_c \delta_c = K^2 (1 - \nu^2) / E = 2\Gamma, \quad (8)$$

where K is the fracture toughness, $E = 2G(1 + \nu)$ is Young's modulus, and Γ is surface energy. After complete separation occurs in either normal or tangential fracture, atomic bonds are considered irreversibly broken, and boundary facets interact subsequently via locally frictionless contact with material interpenetration prohibited [21]. Fracture properties are listed in Table 2 [22, 23].

TABLE 2. Fracture properties for SiC and AlON.

Property	Value (SiC) ^a	Value (AlON) ^b
t_c [GPa]	0.570	0.306
δ_c [μ m]	0.10	0.06
Γ [J/m ²]	28.1	9.0
K [MPa m ^{1/2}]	5.1	2.5

^aReferences [6, 22].

^bReference [23].

MICROSTRUCTURES

In the absence of microstructures from actual test specimens, finite element meshes of synthetic microstructures are used. Polyhedral grain geometries are produced using a Monte Carlo grain growth algorithm [24]. Volume meshes of tetrahedral elements are created from stereolithographic (STL) files of surface representations of grains comprising a given polycrystal [20].

TABLE 3. Features of polycrystalline microstructures.

Feature	Microstructure I	Microstructure II
Dimensions	1×1×1 mm ³	1×1×1 mm ³
No. grains	50	126
Grain size	270 μ m	200 μ m
No. elements	1.59×10 ⁶	1.13×10 ⁶

Two microstructures are considered, with features listed in Table 3. Material properties of SiC or AlON are assigned to either microstructure in a given simulation. In this way, effects of elastic and fracture properties on the overall response are studied while keeping the microstructure (i.e., mesoscale geometry) fixed. Loading in different directions provides an indication of effects of grain structure on anisotropy. Furthermore, different sets of random initial lattice orientations are assigned to polycrystals among different simulations, enabling quantification of effects of anisotropic elasticity.

NUMERICAL SIMULATIONS

Lagrangian finite element calculations are performed using the SIERRA explicit dynamics code [21]. Considered first are results for uniaxial strain compression. A uniform velocity gradient is assigned as an initial condition. The applied strain rate is $\dot{\epsilon} = 10^5/\text{s}$. Under these conditions, the current volume V of the specimen is related to its initial volume V_0 via

$$V = V_0(1 - \dot{\epsilon}t). \quad (9)$$

Figure 1 shows axial stress in a SiC specimen at 6% compression.

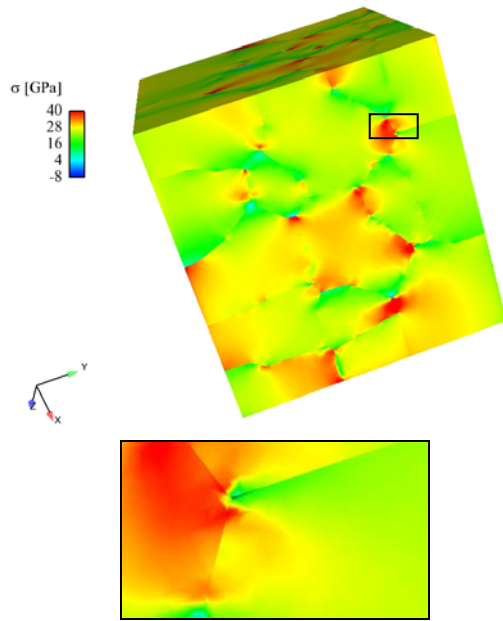


Figure 1. Axial Cauchy stress (positive in compression), microstructure I, SiC, uniaxial strain, $V/V_0 = 0.94$.

In uniaxial strain simulations, one face of the microstructure is assigned a constant velocity in the compression direction while lateral faces are restricted from expanding or contracting. Evident are stress concentrations near grain boundaries and axial splitting cracks typical of brittle materials with low Poisson's ratio [25]. Figure 2 shows average axial stress Σ computed for representative simulations with nonlinear or linear elasticity as

$$\Sigma = \frac{1}{A} \left| \int t^{(n)} dA \right|, \quad (10)$$

where $t^{(n)}$ is the component of traction normal to the compressed face of the microstructure with area A . Also shown for comparison are experimental plate impact data [26-29]. Linear elasticity gives smaller normal stress than corresponding nonlinear models. Figure 3 shows average shear stress

$$\tau = \frac{1}{2} |\Sigma_1 - \Sigma_3|, \quad (11)$$

with $\{\Sigma_1, \Sigma_3\}$ the {maximum, minimum} principle stresses computed similarly to (10). Predictions for SiC are generally lower than experiment; those for AlON are generally closer to experimental data.

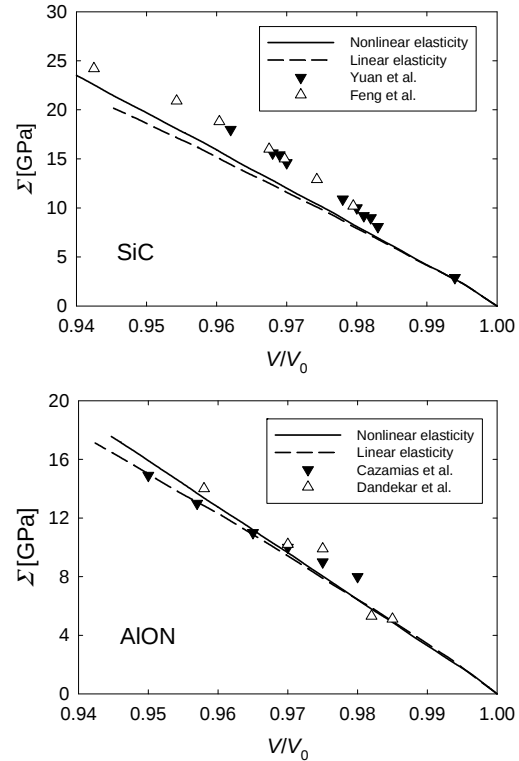


Figure 2. Average axial stress, uniaxial strain.

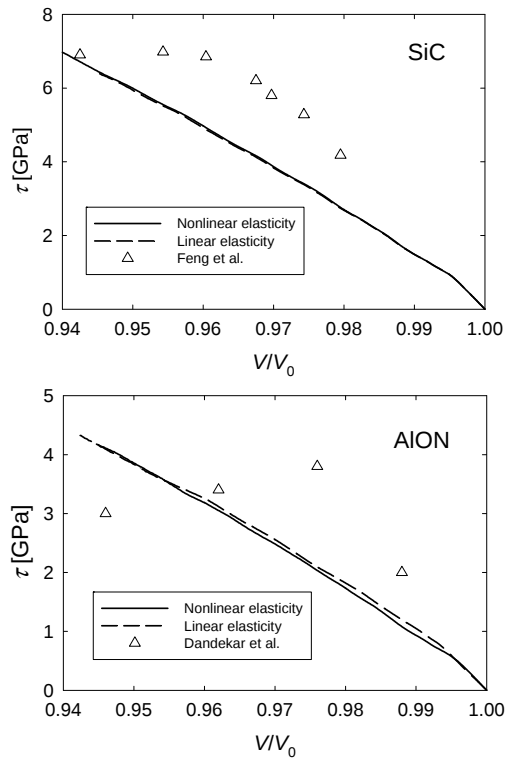


Figure 3. Average shear stress, uniaxial strain.

Unconfined compression simulations are also performed on SiC and AlON microstructures, with initial lattice orientation distributions and loading axes varied among simulations. These and all subsequent results incorporate nonlinear elasticity. Boundary conditions again correspond to a strain rate of $\dot{\epsilon} = 10^5/s$, with a uniform initial velocity gradient prescribed. Peak compressive stresses Σ_x , computed as in (10), are compared with Kolsky bar data [30-32] in Table 4. Again, predictions for AlON are closer to experimental data; however, loading rates in experiments ($\sim 10^3/s$) are smaller than those applied in the numerical simulations.

TABLE 4. Unconfined compressive strength Σ_x [GPa].

	SiC	AlON
Model	4.2-4.9	3.1-3.8
Experiment	5.0-8.2 ^a	3.0-4.0 ^b

^aReferences [30, 31]. ^bReference [32].

Shear simulations are also performed on SiC and AlON microstructures, with initial lattice orientation distributions and loading planes and directions varied among simulations. Boundary

conditions provide a shear strain rate of $\dot{\gamma} = 10^5/s$, with a uniform initial velocity gradient prescribed. In some simulations, all faces are free to expand laterally to accommodate dilatation; in others, the face on which the shear traction is applied is prohibited from expanding, thereby increasing the confining pressure that resists dilatation and impedes shear [2-4]. The former conditions are labeled “free”; the latter are labeled “confined.” Figure 4 shows the shear stress component conjugate to the applied strain rate component in representative simulations. Local shear stresses are higher for confined boundary conditions; similar trends are observed for average shear stresses.

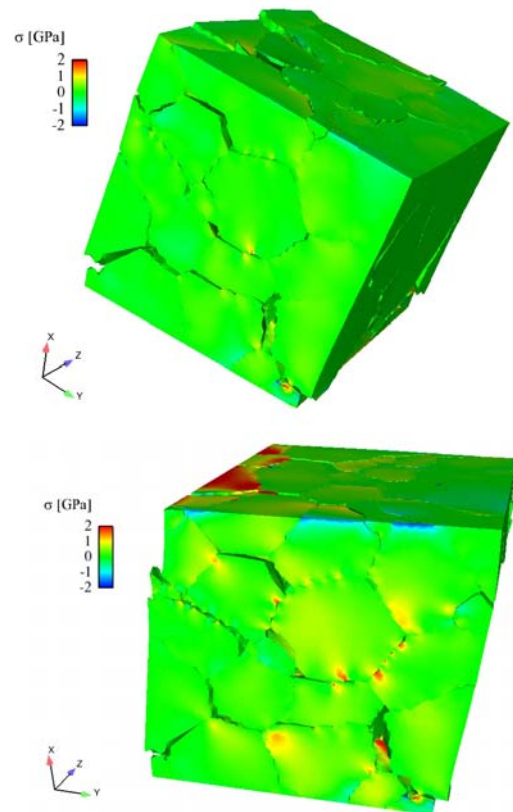


Figure 4. Shear stress, microstructure II, AlON, $\gamma = 0.03$, displacements magnified 5x: unconfined shear loading (upper image), confined shear loading (lower).

Failure statistics from numerous unconfined shear simulations (24 for SiC; 19 for AlON) are now analyzed. Average shear stress τ is computed analogously to (10) for a given polycrystal:

$$\tau = \frac{1}{A} \left| \int t^{(t)} dA \right|, \quad (12)$$

where $t^{(t)}$ is the tangential component of traction applied along A . Shear strength is the (peak) value of τ at which $\partial\tau/\partial\gamma=0$. Table 5 shows normal (i.e., standard Gaussian) statistics computed from discrete values of τ predicted for each material from simulations. The mean value of τ is denoted by $\bar{\tau}$, standard deviation (square root of the variance) by S . Mean strength is lower in AlON than SiC, presumably a result of its lower cohesive strength, surface energy, and elastic stiffness. Standard deviation is larger in AlON than SiC, possibly a result of greater anisotropy and smaller fracture strength and energy that render AlON more sensitive to cracking at grain boundaries or triple junctions favorably oriented for fracture.

TABLE 5. Normal statistics: unconfined shear strength.

Model	SiC		AlON	
	$\bar{\tau}$ [GPa]	S [GPa]	$\bar{\tau}$ [GPa]	S [GPa]
Model	0.511	0.013	0.333	0.027

Table 6 lists Weibull statistics for values of τ predicted from simulations; shown for comparison are statistics from static flexure experiments on much larger specimens [5, 34]. A cumulative Weibull distribution predicts probability f of failure at or below a given shear stress τ as

$$f(\tau) = 1 - \exp[-(\tau/\tau_0)^m], \quad (13)$$

with nominal strength τ_0 and Weibull modulus m . Larger m corresponds to lower variability. Weibull parameters are computed from discrete data points by linear fitting to $\ln\{\ln[1/(1-f)]\}$ versus $\ln\tau$, e.g., following [33]. Predictions for SiC exhibit lower variability and greater nominal strength than those for AlON, in qualitative agreement with experiments. However, because the mesoscale models do not incorporate initial flaws or spatially variable fracture properties, the present results may under-predict variability.

TABLE 6. Weibull statistics: unconfined shear strength.

	SiC		AlON	
	τ_0 [GPa]	m	τ_0 [GPa]	m
Model	0.52	45.2	0.35	14.9
Experiment	0.37- 0.62 ^a	4.9- 26.6 ^a	0.29- 0.81 ^b	2.9- 26.3 ^b

^aReference [5] ^bReference [34]

CONCLUSIONS

Mesoscale models incorporating nonlinear anisotropic elasticity and cohesive fracture have been used to study dynamic compression and shear of SiC and AlON ceramics. Average stresses predicted for compression are in reasonable agreement with experiments on much larger samples of material; agreement between model and experiment is generally closer for AlON than SiC. Predictions for dynamic unconfined shear strength demonstrate greater variability for AlON than SiC, in qualitative agreement with experimental static fracture statistics.

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