Trans and inter-granular peridynamic fracture in polycrystalline ceramics

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June 12, 2008

peridynamics, polycrystalline ceramics, transgranular fracture, intergranular fracture, meshfree methods.

Abstract

1 Polycrystal fracture

1.1 Computational modeling of fracture in polycrystalline materials

One of the main mechanisms through which ceramic materials fail under mechanical loading is brittle fracture. In order to predict the performance and structural integrity of such materials, a fundamental understanding of brittle fracture in polycrystalline ceramics at the grain-size level is required. Such an understanding can then be used to design advanced structural ceramic systems with increased impact resistance, higher thermal shock resilience, etc. Here we present a novel approach for simulating fracture in polycrystalline ceramics, which has been difficult to do in the past, due to, in no small measure, the complexity of the phenomenon.

Combined transgranular (cracks pass through the grains) and intergranular (cracks propagate between the grains) fracture can take place in brittle fracture of ceramics. A transition between the trans- and intergranular fracture is observed under certain conditions of loading rates when the crack starts running unstable. Experiments reported in [1] show the dependence of fracture characteristics of silicon nitride ceramics, on the existence of crystalline phase at triple junctions. While the observed that the main fracture mode is intergranular [1], local transgranular fracture also appears due, apparently, to the existence of crystalline phase at grain junctions. Also, crack deflection and crack bridging mechanisms were observed due to the presence of large, rod-like grains. Further evidence of the importance of accurate modeling of inter- and trans-granular fracture in polycrystalline ceramics is presented by [2] who investigate a theoretical model of intragranular particle residual stress strengthening. The SiC nanoparticles in the Al2O3 grains create a normal compressive stress at the grain boundaries and a tangential tensile stress in the grains, resulting in the "strengthening" of the grain boundaries and "weakening" of the grains. According to the model in [2], there exists an optimum amount of SiC for strengthening, below which the grain boundaries are not fully "strengthened" and the fracture is mainly intergranular, above which the grains are "weakened" too much and the fracture is mainly transgranular, and at which the fracture is a mixture of intergranular and transgranular. Toughening mechanisms in nanocomposites are also reviewed in [3].

Existing models for simulating brittle fracture in polycrystalline ceramics that can include combined trans- and inter-granular crack propagation have severe limitations, including: the inability of modeling propagating cracks that naturally coalesce and/or branch; limitation to modeling only a single or just a couple of cracks; complicated algorithms that cannot extend to 3D, etc. A summary of the existing methods and their limitations is given below.

The FEM has been the preferred tool used in numerical models of polycrystalline materials (see, e.g. [4], [5], [6], [7]. Fracture in polycrystalline materials has been modeled using cohesive-zone models (see below). Cohesive interface modeling of fracture was initiated in [8], [9], [10]. In recent years, cohesive surface models have been widely used to numerically simulate fracture initiation and growth by the finite-element method [11] [12], [13]. Recently, some difficulties regarding time discontinuities in cohesive zone models have been pointed out in [14]. Bias of the crack propagation path and possible remedies are discussed in [15]. Mathematical and physical limitations and constraints on cohesive laws are discussed in, e.g., [16].

In numerical modeling brittle fracture of polycrystalline ceramics the most common approach is to consider *only* intergranular fracture: cracks are restricted to grain boundaries (see, e.g., [17], [18], [6], [19], [20]. In [7], finite elements with a "soft-kill method" are used to propagate the crack along grain boundaries instead of using a cohesive zone model.

Crack propagation behavior in alumina polycrystals is analyzed in [21] using the body force method (BFM) [22] which employs superposition of fundamental solutions. Combined trans- and inter-granular fracture is simulated, but the solutions are based on relations postulated for the mode I to mode II transition and an existing initial crack is postulated. More recently, [23] proposed a two-dimensional XFEM [24] with level sets model for studying the transition from intergranular to transgranular crack growth in polycrystalline materials. It is not clear that this model can be extended to treating multiple cracks in fragmentation scenarios or dynamic problems in 3D.

Lattice spring models have been used to study brittle fracture and damage in polycrystalline materials by, for example, [25], [26]. In the spring network on the lattice, a spring fails if the stored elastic energy in the spring exceeded a critical value. A transition from intergranular to transgranular fracture with increasing grain boundary toughness is observed in [25], however, these studies are limited to 2D quasi-static analysis.

Compared to existing methods, the peridynamic meshfree method used here for analyzing crack initiation, propagation, and fragmentation in a rate-dependent mechanically loaded Voronoi polycrystalline ceramics has important advantages because:

- The cracks initiate and propagate when and where is it energetically favorable to do so;
- Inter- and transgranular fracture are direct consequences of the computations and they do not have to be postulated via ad hoc assumptions as is the case for the classical approach;
- Mode-transition and mode-mixing of crack propagation is naturally captured by the peridynamic formulation;
- Fracture at triple-junction points is not controlled by ad-hoc assumptions but by the actual loading conditions in a region surrounding the triple-junctions;
- Complex interaction between cracks does not have to be assumed, but rather it is part of the solution;
- The meshfree character eliminates the need for complicated meshing algorithms for Voronoi polycrystals, which in 3D are still great obstacles;
- Modeling of initial (residual) strains/stresses, voids, and particle inclusion can be implemented directly.

1.2 Numerical examples of 2D peridynamic models for trans- and inter-granular fracture of polycrystals

The examples we consider here are for polycrystalline silicon. The full details are given in [27]. Single-crystal silicon has a cubic structure, with the elastic moduli $c_{11} = 166$ GPa, $c_{44} = 80$ GPa, and $c_{12} = 64.5$ GPa.

Extensions to other types of crystals or to 3D simulations are immediate and do not require anything special. The directional variation of the "effective stiffness" (ratio of uniaxial stress and extensional strain in the same direction) is shown in Fig. 1. Note that for this type of single-crystal, the effective elastic stiffness varies from 130 GPa to 170 GPa, with the stiffest direction being the 45 degree one.

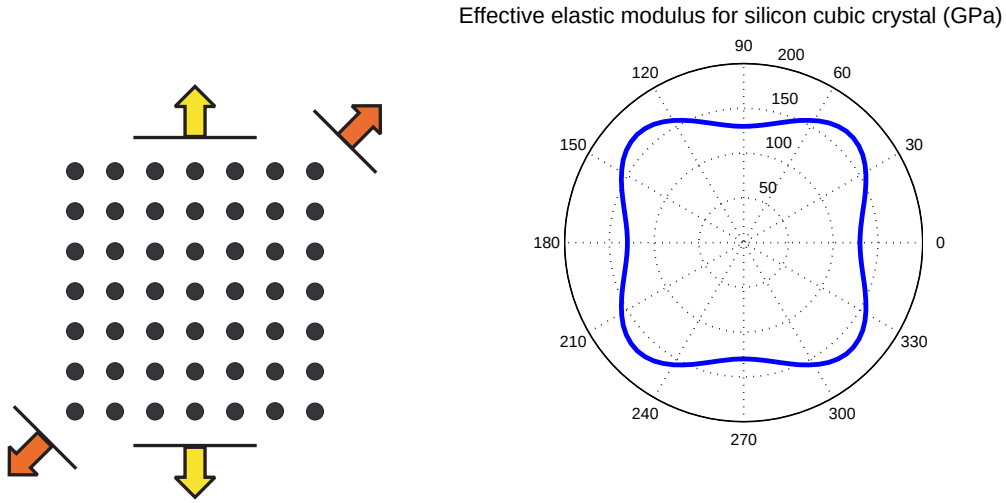

Figure 1: The lattice structure of a cubic crystal. The effective stiffness modulus for the silicon crystal

We generate a Voronoi polycrystal over a square with dimensions of 1cm by 1cm. Using 120 randomly distributed x and y coordinates for the Voronoi cells seeds, we obtain a grain-size distribution that is close to a Weibull distribution. This number of cells in the Voronoi structure gives the same grain-size distribution for different realizations (see [27]). For each Voronoi cell we assign a certain, random, orientation angle (from a uniform distribution). We define the micro-stiffness for the peridynamic bonds to vary with their orientation inside the grain and match the effective stiffness in Fig. 1. Thus, the micro-stiffness depends on the orientation of each grain and the orientation of the bond inside the grain.

The peridynamic bond relative elongation is defined by $s = (\|\mathbf{y}' - \mathbf{y}\| - \|\mathbf{x}' - \mathbf{x}\|)/\|\mathbf{x}' - \mathbf{x}\|$, and the critical relative elongation at which a bond breaks is associated with the fracture energy and the peridynamic horizon via (see [28]) $s_0 = \sqrt{\frac{5G_0}{9\kappa\delta}}$, where G_0 is the material's (single crystal silicon) fracture energy and κ is the bulk modulus. This critical relative elongation may be orientation-dependent, but this is not done here. Moreover, bonds that connect different grains have special properties that may be related to the properties of the grain boundaries. In this study we select the micro-stiffness for such bond to be the average of the corresponding directions in the two grains. For the critical relative elongation of the bonds that have ends in different grains we define an "interface strength coefficient"

$$\beta = \frac{s_0^{\mathrm{GB}}}{s_0}$$

where s_0^{GB} is the critical relative elongation of the bonds that pass over a grain boundary, and s_0 is the value defined above for the single-crystal material. As we vary β from sub-unitary to super-unitary numbers, we change the strength of the grain boundaries from lower than the single crystal to higher than the single crystal.

For the numerical discretization one can use a structured or an unstructured grid (see Fig. 2). In the examples below we show results based on a structured grid of 100 by 100 nodes. The tests are performed using EMU [29]. We apply velocity boundary conditions on two sides for stretching along the horizontal direction. The top and the bottom sides are free. The applied strain rate is constant equal to 50/s and the

initial velocity distribution is consistent with this strain rate. We simulate 32 μs to reach an effective strain of 0.2%. We do not introduce initial cracks.

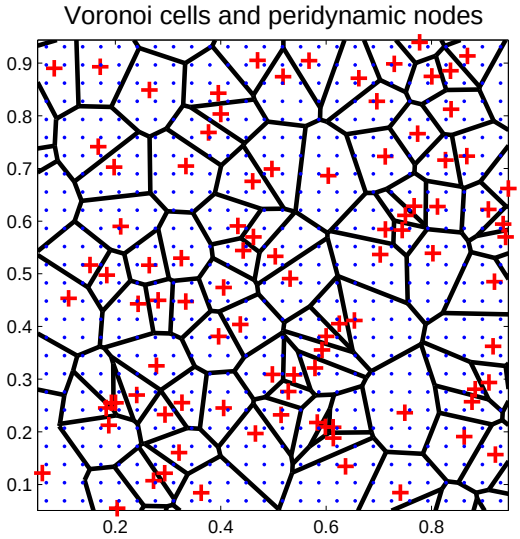

Figure 2: A sample of a peridynamic discretization (structured) for a random Voronoi polycrystal. The peridynamic nodes are in blue, while the Voronoi seeds are shown with the red crosses. The results below are computed on a denser grid of 100 by 100 nodes and a different realization of the Voronoi structure.

The plots in Fig. 3 show the polycrystal after 22 μs of the simulation for different values of the interface strength coefficient β. As β increases from 0.25 (left figure) to 1 (center) to 4 (right figure), we transition between purely intergranular fracture to pure transgranular fracture, passing through combined trans- and inter-granular fracture observed for average values of β.

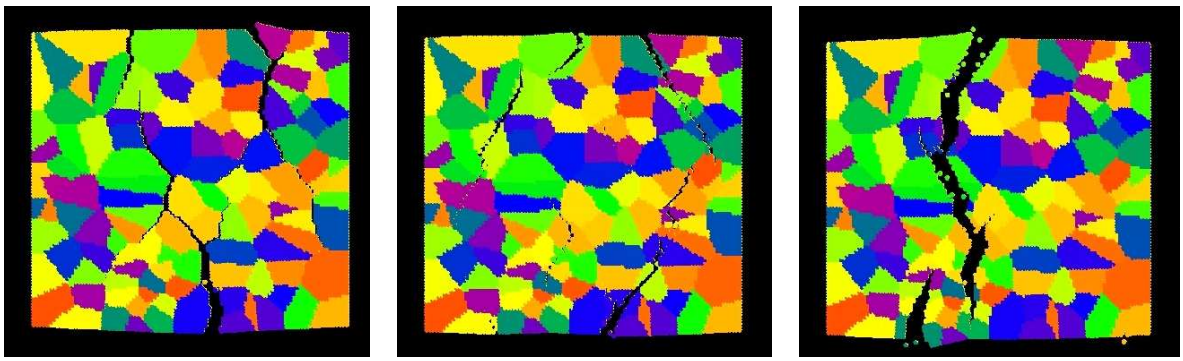

Figure 3: Fracture dependence on parameter β: β=0.25 (left), β=1 (center), and β=4(right). Combined trans- and inter-granular fracture are observed for average values of this grain boundary strength parameter. Note the primarily transgranular for large β and dominant intergranular for small values of β.

To better observe the ability of the peridynamic method to simulate crack propagation and crack interaction in polycrystalline ceramics we monitor the damage time-evolution for the case when $\beta = 1$ (see Fig. 4). We note that there are cracks that begin from the top and bottom edges, but also cracks that start in the interior of the sample, grow, branch, and finally join together.

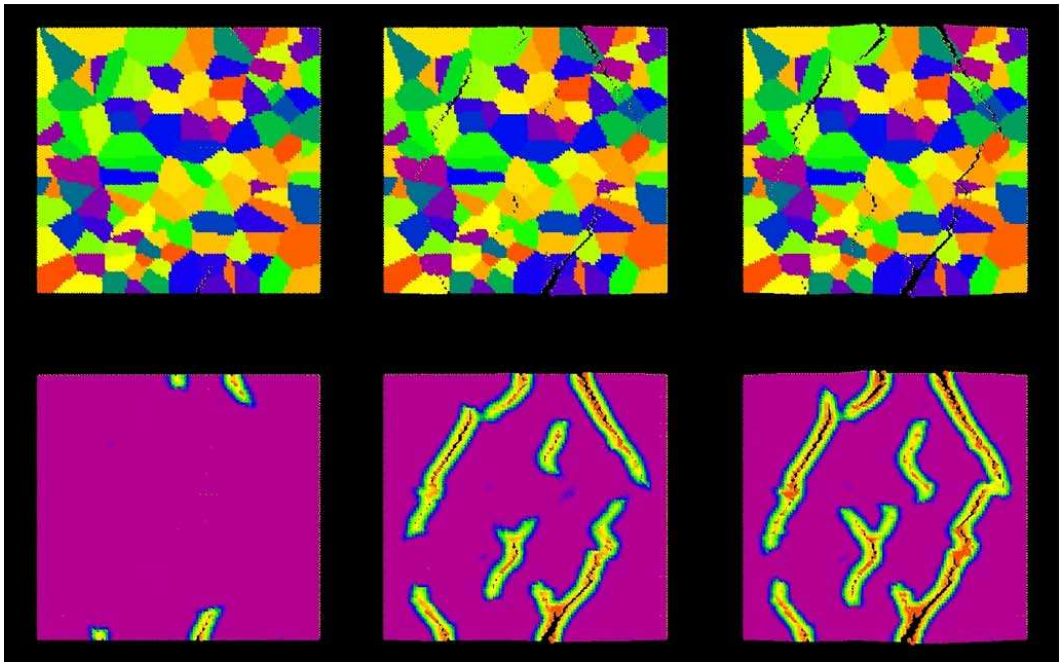

Figure 4: Evolution of damage and cracks in time for the $\beta = 1$ case. The top row show the polycrystals boundaries while bottom row shows the damage index. Notice that cracks branch and coalesce as conditions require, and that trans- and inter-granular fracture take place. Some cracks start in the interior of the sample. The three columns of figures are captured at 20.5 μs, 21.3 μs, and 22.1 μs, respectively.

References

[1] B-T. Lee, B-D. Han, and H-D. Kim. Comparison of fracture characteristic of silicon nitride ceramics with and without second crystalline phase. *Materials Letters*, 58:74– 79, 2003.

[2] X. Sun, G.-J. Li, S. Guo, Z. Xiu, K. Duan, and X.Z. Hu. Intragranular particle residual stress strengthening of al2o3-sic nanocomposites. *Journal of the American Ceramic Society*, 88(6):1536–1543, 2005.

[3] S.-M. Choi and H. Awaji. Nanocomposites - a new material design concept. *Science and Technology of Advanced Materials*, 6(1):2–10, 2005.

[4] S. Ghosh and S.N. Mukhopadhyay. A material based finite element analysis of heterogeneous media involving dirichlet tessellations. *Computer Methods in Applied Mechanics and Engineering*, 104:211–247, 1993.

[5] S. Ghosh and R.L. Mallett. Voronoi cell finite elements. *Computers and Structures*, 50(1):33–46, 1994.

[6] P.D. Zavattieri, P.V. Raghuram, and H.D. Espinosa. A computational model of ceramic microstructures subjected to multi-axial dynamic loading. *Journal of the Mechanics and Physics of Solids*, 49(1):27–68, 2001.

[7] D. Zhang, M.S. Wu, and F. Feng. Simulation of microplasticity-induced deformation in uniaxially strained ceramics by 3-d voronoi polycrystal modeling. *International Journal of Plasticity*, 21:801–834, 2001.

[8] G.I. Barenblatt. The formation of equilibrium cracks during brittle fracture: general ideas and hypotheses, axially symmetric cracks. *Applied Mathematics and Mechanics (PMM)*, 23:622636, 1959.

[9] D.S. Dudgale. Yielding of steel sheets containing slits. *Journal of the Mechanics and Physics of Solids*, 8:100–104, 1960.

[10] G.I. Barenblatt. The mathematical theory of equilibrium cracks in brittle fracture. *Advances in Applied Mechanics*, 7:55–129, 1962.

[11] X.P. Xu and A. Needleman. Numerical simulations of fast crack growth in brittle solids. *Journal of the Mechanics and Physics of Solids*, 42:13971434, 1994.

[12] G.T. Camacho and M. Ortiz. Computational modeling of impact damage in brittle materials. *International Journal of Solids and Structures*, 33:2899–2938, 1996.

[13] M. Ortiz and A. Pandolfi. A class of cohesive elements for the simulation of three-dimensional crack propagation. *International Journal for Numerical Methods in Engineering*, 44:1267–1282, 1999.

[14] K.D. Papoulia, C.H. Sam, and S.A. Vavasis. Time continuity in cohesive finite element modeling. *International Journal for Numerical Methods in Engineering*, 58:679–701, 2003.

[15] R. de Borst. Numerical aspects of cohesive-zone models. *Engineering Fracture Mechanics*, 70:1743–1757, 2003.

[16] Z.H. Jin and C.T. Sun. Cohesive fracture model based on necking. *International Journal of Fracture*, 134(2), 2005.

[17] M. Grah, K. Alzebdeh, P.Y. Sheng, M.D. Vaudin, K.J. Bowman, and M. Ostoja-Starzewski. Brittle intergranular failure in 2d microstructures: Experiments and computer simulations. *Acta Materialia*, 44:4003–4018, 1996.

[18] E.A. Holm. Surface formation energy for intergranular fracture in two-dimensional polycrystals. *Journal of the American Ceramic Society*, 81(3):455–459, 1998.

[19] S. Maiti and P.H. Geubelle. Mesoscale modeling of dynamic fracture of ceramic materials. *Computer Modeling in Engineering and Sciences*, 5:91 – 101, 2004.

[20] S. Maiti, K. Rangaswamy, and P.H. Geubelle. Mesoscale analysis of dynamic fragmentation of ceramics under tension. *Acta Materialia*, 53:823 – 834, 2005.

[21] B.-N. Kim, S. Wakayama, and M. Kawahara. Characterization of 2-dimensional crack propagation behavior by simulation and analysis. *International Journal of Fracture*, 75:247–259, 1996.

[22] H. Nisitani and D.H. Chen. Body force method and its applications to numerical and theoretical problems in fracture and damage. *Computational Mechanics*, 19:470–480, 1997.

[23] N. Sukumar, D.J. Srolovitz, T.J. Baker, and J.-H. Prevost. Brittle fracture in polycrystalline microstructures with the extended finite element method. *International Journal for Numerical Methods in Engineering*, 56(14):2015–2037, 2003.

[24] N. Mos and T. Belytschko. Extended finite element method for cohesive crack growth. *Engineering Fracture Mechanics*, 69:813–833, 2002.

[25] W.H. Yang, D.J. Srolovitz, G.N. Hassold, and M.P. Anderson. *In Simulation and Theory of Evolving Microstructures*, chapter Microstructural effects in the fracture of brittle materials, pages 277–284. The Metallurgical Society: Warrendale, PA, 1990.

[26] A. Rinaldi, D. Krajcinovic, P. Peralta, and Y.-C. Lai. Lattice models of polycrystalline microstructures: A quantitative approach. *Mechanics of Materials*, 40:17–36, 2008.

[27] F. Bobaru and S.A. Silling. Trans and inter-granular peridynamic fracture in polycrystalline ceramics. *in preparation*, 2008.

[28] S.A. Silling and E. Askari. A meshfree method based on the peridynamic model of solid mechanics. *Computers and Structures*, 83(17-18):1526 – 1535, 2005.

[29] S. A. Silling and E. Askari. A meshfree method based on the peridynamic model of solid mechanics. *Comp. Struct.*, 83:1526–1535, 2005. EMU available at http://www.sandia.gov/emu/emu.htm.