Revealing microstructural parameters influencing strength and toughness of silicon nitride

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ABSTRACT

Discovering microstructural features which influence macroscopic properties has appealed to many researchers. In many materials (including silicon nitride), a slight change in microscopic properties can bring a huge difference in their macro-scale behavior, increasing the number of potential industrial applications. Materials scientists are able to monitor the grain size, the amount of porosity and of second phase material within silicon nitride, which alters the macro-scale toughness and strength. There is a strong interest in developing robust numerical methods for simulating damage mechanisms in this material. In this paper, we study the influence of needle-shaped grains, which are found in silicon nitride, on mechanical strength and toughness. This calls for addressing the numerical challenge of capturing both its intergranular and transgranular cracking, a topic which has been overlooked in the literature [3].

We present a two-dimensional finite-element framework for modeling silicon nitride at the microscale. The microstructure is constructed using a Voronoi tessellation, in which a clustering technique was used to append a given needle-shaped grains density. The cohesive element framework developed by Dugdale [2] is utilized for considering fracture within the microstructure. We resort to the cohesive law proposed by Camacho [1] for modeling crack opening, whereas the bulk behavior is considered as isotropic and elastic. As in the hexagonal structure of Si_3N_4 grains, cleavage planes have an angle of 60 degrees with one another [4], we generated a discretization which was aligned with those randomly oriented planes (see figure 1), all the while keeping a sufficient mesh quality.

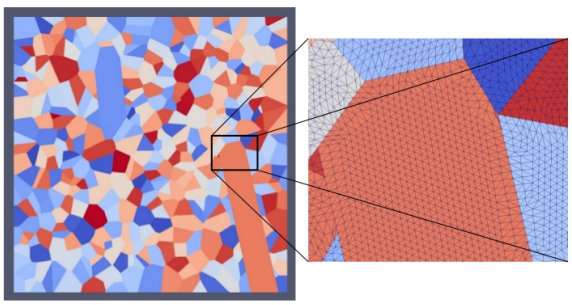

Figure 1: Silicon nitride microstructure whose elements are aligned with cleavage planes

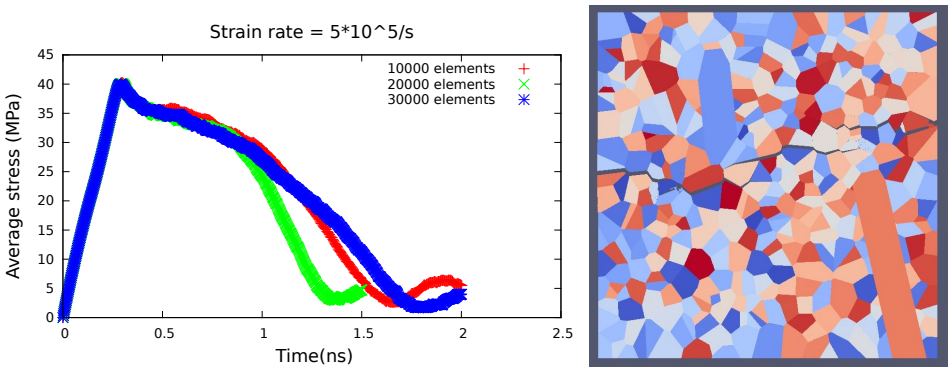

Figure 2: Studying the mesh convergence of our approach

Consequently, the discretization which consists of equilateral elements could be utilized to denote the crystal structure of the grains. This original approach for transgranular cracking does not require (a computationally intensive) remeshing procedure and data transferring for aligning the elements with cleavage planes. This allows the study of much larger microstructures than was done in [3]. It also should be mentioned that the number of cracks inside a grain is not limited. The cohesive properties for intergranular and transgranular cracking were gathered in the literature and given some randomness to capture the microstructural diversity in grain boundaries and material defects.

We first present results concerning mesh dependency. Consequently, we chose a microstructure with three different discretizations, but under the same loading conditions (strain rate= tensile, ...). As it is shown in figure 2, the same strength was obtained for all three microstructures. Moreover, the final amounts of dissipated energy have a satisfactory agreement, although we do not expect an exact match due to the randomness in fracture parameters. Several physical parametric studies were performed. In particular, the calculations reveal a strong rate dependence in the presence of needle shapes. Increasing the strain rate yields higher dissipated energy and higher strength. We observe as well that it increases the percentage of trans-granular fracture (which in conjunction to a broader crack network, is one of the reasons for the observed strain rate hardening). In another parametric study, the microstructure was varied. We show that when needle grains are more numerous and coarser, the specimen's toughness increases. A detailed examination of the crack paths reveals that needles cause more deflections, which increases the material's resistance to crack propagation, but also increases the probability of trans-granular fracture.

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