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ScienceDirect

Acta Materialia 67 (2014) 239–251

Acta MATERIALIA

www.elsevier.com/locate/actamat

On the influence of transgranular and intergranular failure mechanisms during dynamic loading of silicon nitride

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Received 27 August 2013; received in revised form 19 December 2013; accepted 20 December 2013
Available online 1 February 2014

Abstract

Plane-strain tensile loading numerical simulations of dynamic crack propagation in silicon nitride microstructures are conducted. The strength and toughness are evaluated as a function of strain rate and microstructural parameters, including grain size and density of needle-shaped grains. The silicon nitride microstructures are built using Voronoi tessellation for constructing regular grains and a merging procedure to generate elongated grains. Dynamic insertion of cohesive elements representing transgranular and intergranular cracking is a key feature of the modeling. The results show that inertia and elongated grains both contribute to the rate hardening of the specimen. The simulations reveal the existence of a threshold opening rate for intergranular cracks to transform into transgranular ones. Moreover, a higher percentage of transgranular fracture causes higher toughness.

Keywords: Microstructural parameters; Dynamic loading; Transgranular and intergranular cracking; Cohesive elements

1. Introduction

Experimental observations of strong variability in the strength and toughness of ceramics under dynamic loading inspired many researchers to look for microscopic origins. Microstructural complexity hampers our comprehension of the physics underlying damage mechanisms. In the case of silicon nitride, this complexity arises from two different populations of grains: regular and needle-shaped grains, coming from α and β phase seeds, respectively (see Fig. 1a). Besides grain size, the presence of an amorphous glassy phase material and porosity can affect the micro-damage mechanisms. These microstructural features are produced by the sintering process. In addition, under high tensile stress fields, microcracks originate from two competing damage mechanisms, which are intergranular (i.e. at the grain boundaries) and transgranular cracks (i.e. through the grains).

Several experiments have been conducted to study the influence of the microstructural parameters on the macroscopic response and alternatively to study microscopic outcomes owing to macroscopic boundary conditions [1–3]. More specifically, Kleebe et al. [4] tried to determine the effects of grain morphology and a second-phase material on the fracture toughness of silicon nitride. They observed an increase in fracture resistance with increasing grain diameter. Moreover, Sun et al. [5] studied the effects of the size and shape of grains on the fracture toughness. They concluded that the fracture resistance increases greatly with a distinct bimodal distribution of grain diameters. They also found that unreinforced (i.e. no needles) equiaxed silicon nitride exhibits the lowest toughness compared to other microstructural morphologies. Furthermore, Li et al. [6] attempted to find how the strength of a

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1359-6454/$36.00
http://dx.doi.org/10.1016/j.actamat.2013.12.032

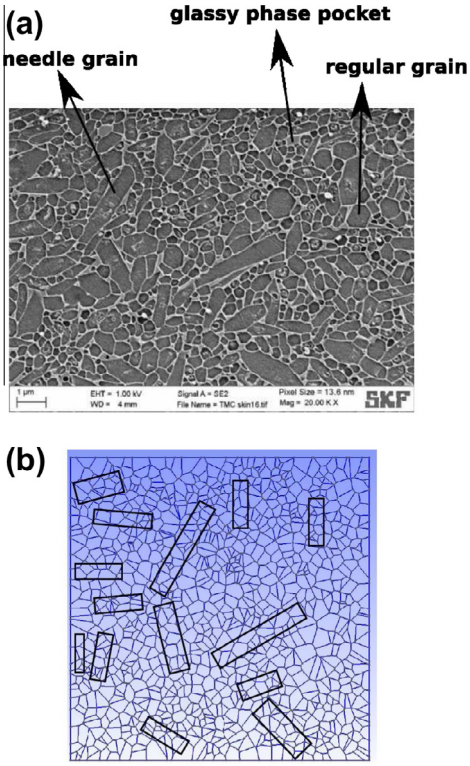

Fig. 1. (a) Example of a silicon nitride microstructure. (b) Merging grains inside boxes for creating needle-shaped grains.

specimen varies by changing the microstructure. They provided an explanation for the toughening behavior using an elastic bridging model for short cracks and a pull-out model for long cracks. The relation between different grain-type densities and mechanical properties was studied by Xu et al. [7]. They found that the mechanical properties have an optimum region where the α/β ratio is equal to 1. They concluded that both flexural strength and fracture toughness can be improved by controlling the population, aspect ratio and size distribution of rod-like grains. In yet another investigation, Hu et al. [8] observed that the percentage of transgranular fracture increases by raising the strain rate. Although all of these experiments have the advantage of revealing real data, they have limited control on the input parameters and output data. Therefore, numerical simulations are necessary to complement the experimental interpretations by specifying the underlying physics. It can also help assess the accuracy of experimentally measured parameters and explore the influence of a wide range of parameters.

Cohesive zone modeling is arguably the most popular method for modeling dynamic crack propagation. The theoretical basis of this model was developed by Dugdale and Barenblatt [9,10]. Finite element implementation (cohesive elements) was pioneered by Xu and Needleman [11] and Camacho and Ortiz [12]. The success of the method has spread its use to several applications, including fragmentation [13,14], mixed-mode damage in concrete [15], thermo-mechanical applications [16] and modeling dynamic crack growth at interfaces [17]. The use of cohesive elements for modeling crack propagation in ceramics has been reported in several investigations. Kraft and Molinari [19,18] studied the effects of grain boundary properties on intergranular and transgranular fracture. The limited number of grains that could be modeled in their microstructures (around 30) did not allow the representation of needle-shaped grains. Zhou and Molinari [20,21] investigated the stochastic fracture of ceramics under dynamic tensile loading. Maiti et al. [14] showed the basic features of the fragmentation process, such as the initiation time and the evolution of the fragment size distribution. They also quantified the effect of the failure strength on the initiation and extent of damage. Moreover, Yu et al. [22] proved that simulations can give accurate values for the dynamic strength of six different ceramics. They also predicted the main features of the crack patterns. Despite these numerous investigations, cohesive elements have been criticized for having a strong mesh dependency. The cracks are doomed to propagate along existing element boundaries unless adaptive meshing is performed. Therefore, some other approaches, such as meshless methods, continuum damage approaches and also the extended finite element method (XFEM) have been proposed [23–25]. However, it should be noted that these methods have drawbacks, such as difficulty in handling free surfaces for meshless methods, difficulty in identifying material parameters for continuum damage methods, and the complexity and use of ad hoc parameters in crack branching and coalescence cases with XFEM. Thus, in this research, we use the cohesive element method for modeling cracks. In particular, we resort to dynamic insertion of cohesive elements [12]. For the simulations envisioned in this study, mesh dependency is not a fundamental issue, as cracks are guided by the microstructure and cleavage planes, which we will model explicitly. It should be noted that in this paper, we use a 2-D microscopic model. This implies several restrictions. For instance, out-of-plane motions do not exist. Moreover, the crack network and cleavage planes are in reality three-dimensional. Although extension to 3-D simulation is a necessary future step to obtain quantitative results, we believe that relevant qualitative information can be captured by performing 2-D simulations.

To the best of our knowledge, only a few authors have conducted simulations on a silicon nitride microstructure containing elongated grains. A notable example is the work of Wippler and Boehlke [29,26,28,27], in which they studied the thermoelastic and fracture properties of this material. In their study a phenomenological model is used to consider the microcracks without representing explicit crack surfaces. They also performed a limited set of parametric studies on the size and aspect ratio of grains.

The aim of this paper is to investigate the effect of intergranular and transgranular cracking mechanisms in view of microstructural features of Si_3N_4, such as grain size and density of needle-shaped grains. We will also look into the microstructural origins of strain rate hardening.