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Micromechanical simulation of fracture behavior of bimodal nanostructured metals

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ABSTRACT

Nanostructured (NS) metals with bimodal grain size distribution that consist of coarse grained (CG) and nano-grained (NG) regions have proved to have both high strength and good ductility. In this paper a numerical investigation, using the combination of a mechanism-based strain gradient plasticity theory, a micromechanics composite model, and the Johnson–Cook failure model, is conducted to investigate the effects of the distribution of the CG inclusions and their shape on fracture behavior of a bimodal NS copper. Load–response relations are employed to evaluate the loading history stability, while apparent crack length and strain energy history are used to analyze the fracture resistance. This study shows that both crack bridging in the CG inclusions and crack deflection in the NG matrix can significantly toughen the bimodal NS Cu. Our simulations also show that there exists a critical volume fraction of CG inclusions for some microstructures at which the fracture resistance of the bimodal NS Cu is at its minimal state and thus it should be avoided in material design.

1. Introduction

Nanocrystalline metals are known to have high yield stress but they generally lack good ductility. In recent years nanostructured (NS) metals with bimodal grain size distribution, by mixing up the length scales with nano-grained (NG) or ultrafine-grained (UFG) regions as the matrix phase and coarse grained (CG) regions as toughening inclusions, have shown high yield stress and large gain in work hardening and failure strain. The bimodal concept is now a viable way for new material processing and design aimed at both high strength and high ductility.

Many experimental efforts have been devoted to study fracture behavior and toughening mechanisms of the bimodal NS metals. Compared with the strongest commercialized Al alloy, bimodal NS Al alloy had a 30% increase in strength and no loss in ductility due to the presence of the CG zone [1]. A bimodal NS Cu exhibited a failure strain of about 65% and yield stress that is several times of its CG counterpart [2]. As volume fraction of the CG inclusions increased, the ductility of bimodal NS Al alloy was found to increase due to crack bridging and the debonding between NG and CG regions [3]. In general bimodal grain size distribution can be produced by consolidating a simple mixture of powders of different grain sizes and, depending on the microstructural variations, a wide range of property improvement could be achieved [4–6]. Equally intriguing, NS Al sub-micrometer thin films were found to become ductile due to the bimodal grain distribution [7]. In bimodal UFG Al–Mg alloy the CG region was also found to contribute to their overall ductility [8]. The CG could bridge surfaces of cracks originating in the NG regions so that bimodal Ti samples tended to exhibit lower strength but enhanced ductility as compared to NG and UFG Ti [9,10]. By modifying grain size distribution in a multimodal grain structure in Ti, a combination of high yield stress and large uniform elongation has also been reported [11]. The CG bands could also arrest cracks by local blunting, resist crack propagation by bridging, and impede crack propagation by crack deflection, branching, and debonding [12]. The same mechanisms also worked in bimodal UFG Al–Mg alloy and it was found that increasing the volume fraction of the CG regions could increase the ductility with only a slightly-reduced strength [13]. Large localized plastic strain within the CG in the bimodal UFG Ni alloy could also lead to strain localization and debonding [14].

Even with these promising observations, it must be recognized that direct experimental measurement still has its intrinsic limitations. Specifically the exact grain size distribution, grain shape, and

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arrangement, which depend on the fabrication processes, are difficult to reproduce, and the overall mechanical responses hence become tricky to predict [4]. There is very limited theoretical modeling and numerical investigation on fracture behavior of bimodal NS metals. Among these limited studies, we have found that a unit-cell model was used in [15] to study the failure process in a bimodal NS Al alloy, but in the study only one set of yield stress and tensile strength of the NG was extracted from experiments. There was a lack of reliable constitutive relations for the NG phase. As a consequence systematic quantification of the important factors in the fracture behavior of the bimodal NS metals could not be carried out. In another study it was reported that there was initiation of nanocracks at the boundaries between the CG and NG regions, and indicated that good ductility came from the CGs in suppressing the crack growth and providing strain hardening [16]. A micromechanical model of dual-phase composite showed that smaller ductile particles favored not only uniform elongation but also the overall strength, resulting from the higher strain hardening ability of the CG inclusions [17]. But numerical investigations which could address the effects of inclusion distribution and its shape on the fracture behavior of bimodal NS metals still remain unavailable in the literature. This observation has motivated us to undertake this study.

In this paper, the mechanism-based strain gradient plasticity theory will be adopted to describe the constitutive relation of the NG phase and the Johnson–Cook plasticity model will be employed to describe the constitutive relation of each phase at high strain rate. In addition, a micromechanics composite model will be incorporated into this bimodal framework. The dependence of fracture resistance on a series of important factors, including the NG grain size, and microstructure and volume fraction of the CG phase, will be fully analyzed. Our computational investigation will focus on how the toughening mechanisms work in such a diverse microstructure environment so that the key factors which could serve to improve its strength and ductility could be identified.

2. Problem statement and numerical framework

2.1. Specimen configuration and idealized microstructures

A center-cracked tension bimodal NS Cu specimen is studied. It has a width 2.0 mm, a height 0.6 mm, and a pre-crack with a length 0.44 mm. Only one-half of the specimen is used due to symmetry, as shown in Fig. 1. The microstructure in a small region ($60 \times 300\ \mu m^2$) in front of the pre-crack tip is taken into consideration. Fig. 1 also illustrates finite element discretization and a sampled idealized microstructure of the bimodal NS Cu, with the NG phase in green and the CG phase in red. The material outside the microstructure is assumed homogeneous, whose properties are determined by a micromechanics composite model in Section 2.3. Fine meshes are used to resolve an intense stress field and a detailed fracture process. Specifically, linear triangular elements [18] with each size in the order of 1 μm are used in the microstructure region. The number of nodes is about 235 k and that of triangular elements about 468 k. Note that the mesh size cannot resolve individual grain, grain boundary, and orientation of both the NG and the CG phases. Therefore, these two phases will be represented by homogenized constitutive relations, as described in Section 2.2 below.

The morphological parameters of the actual bimodal NS Cu are influenced by the microstructures. To study the influences of phase attributes, six idealized microstructures are considered, as shown in Fig. 2. The volume fraction of the CG Cu inclusions is 24.5% on average, while the arrangement and shape vary. Microstructures A and C (Fig. 2a and c) consist of regular arrays of uniform regions

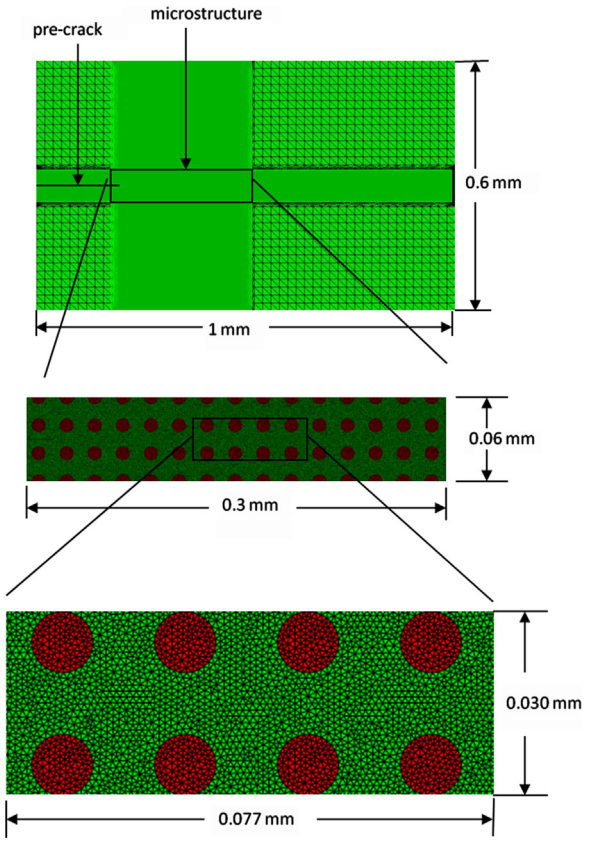

Fig. 1. Finite element discretization and a sampled microstructure of bimodal NS Cu. (For interpretation of the references to colour in this figure, the reader is referred to the web version of this article.)

with square unit cells. Microstructures B and D (Fig. 2b and d) have a staggered region arrangement. The circular regions in microstructures A and B have a radius of 5 μm. The square regions in microstructures C and D have the same area with the circular ones in microstructures A and B, respectively. It should be recognized that square CG inclusions embedded in an NG phase are difficult to achieve experimentally, but they could serve as approximations to the irregular or faceted morphology of the CG phase. But particles with almost square shape have been reported for Bi_2WO_6 products [19]. Microstructures E and F have randomly-distributed unidirectional elliptical regions with half-major and half-minor axes 10 and 2.5 μm, respectively, resulting in an aspect ratio of 4. In microstructure E (Fig. 2e), the direction of the pre-crack path is aligned along the major axis, while in microstructure F it is perpendicular. It may be noted that random arrangement of the elliptical CG inclusions with aspect ratio 4 is consistent with experimental observations of some typical bimodal microstructures such as as-extruded Al–Mg alloy with CG 30% [12]. Elliptical inclusions have also been reported in other types of material systems [20].

Here, the specimen is initially stress free and at room temperature. Tensile load is applied by imposing symmetric velocity boundary conditions along the upper and lower edges of the specimen. The upper boundary velocity is 1 m/s, corresponding to the overall strain rate $3.3 \times 10^3\ s^{-1}$. Symmetric boundary condition is applied to the left edge since only half of the center-cracked specimen is used in the simulation, and the right edge is traction free. Condition of plain strain is assumed to prevail.

2.2. Constitutive relation of the NG phase

The volume fraction of grain boundary increases significantly in the NG phase and its influence on the deformation needs to be