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### Study of deformation and ductile fracture behaviors in micro-scale deformation using a combined surface layer and grain boundary strengthening model

### W.T. Li<sup>a</sup>, M.W. Fu<sup>a,b,\*</sup>, S.Q. Shi<sup>a</sup>

<sup>a</sup> Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong <sup>b</sup> PolyU Shenzhen Research Institute, No.18 Yuexing Road, Nanshan District, Shenzhen, PR China

#### ARTICLE INFO

Keywords: Constitutive model Grain size effect Ductile fracture Stress triaxiality Micro-scale deformation

#### ABSTRACT

A constitutive model considering the composition of surface grain, grain boundary and grain interior and their contributions to the flow stress or strength of materials in micro-scale plastic deformation is developed and termed as a combined surface layer and grain boundary strengthening model in this research. To determine the composition of the three interior microstructural parts of materials, optical microscope and digital image processing technologies are employed. A series of micro-tensile experiments using the specimens with three different geometrical shapes and microstructural grain sizes are conducted for study of deformation and ductile fracture behaviors of material. The model is implemented in finite element analysis and validated via physical experiments. The relationship among fracture strain, grain size and stress triaxiality of the deforming material is thus established. It is found both fracture strain and stress triaxiality increase with the decrease of grain size, while the high stress triaxiality leads to small fracture strain for the given grain size. Through observation of the fractographs, it is revealed that the domination of shear fracture in the 'cup-cone' fracture increases with grain size. The research thus helps understand the ductile fracture in micro-scale deformation and facilitates deformation based working process determination and application.

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#### 1. Introduction

Nowadays, micro-scale parts have been widely used in many industrial applications such as consumer electronic, watch and jewelry, biomedical devices and system, and micro-electro-mechanical system (MEMS), etc. and they are increasingly demanded due to newly emerging requirements from different aspects such as material and energy saving, weight and volume decreasing, environmental impact reducing and product portability increasing [1,2]. To produce micro-scaled metallic parts on a large scale, deformation based micro-manufacturing is one of the efficient approaches. In this process, ductile fracture (DF) is a critical phenomenon to be considered as it affects the geometry and shape of forming of micropart and its quality and property tailoring. DF is thus critical in design of fracture resistant process, determination of the formability of material and quality assurance of defect-free parts [3-5]. DF in micro-scale deformation process, on the other hand, differs from that in macro-scale mainly due to the size effects arising from different sources including variation of material geometry size and microstructural grain size on the deformation behavior, material flow, surface quality, shape accuracy, dimension accuracy and defect formation [6,7]. In-depth understanding of the fracture mechanism, mode and behavior of DF would facilitate the development of deformation based micro-manufacturing process.

DF and the deformation exist simultaneously in the deformation based working process of materials. Both need to be extensively considered concurrently for exploring DF in micro-scale. Some researchers have made their efforts to address this issue in the past few decades. To name a few, a mixed constitutive model built on the surface layer model by combining the theories of single-crystal and polycrystal was established by Lai et al. [8]. In their model, the properties of single-crystal and polycrystal almost represent those of surface and inner grains, respectively. A new composite model employed to show the impact of dimension, shape and grain size of specimen on plastic deformation was built by Shen and Yu [9]. They concluded that the decrease amount of the strength of material is slowly increased with the decreased billet dimension and the increased grain size. The section shape of billet plays a critical role on it as well. The decrease amount of the strength of billet with circular cross-section shows smaller than that of billet with rectangular cross-section in the same section area. According to the composite model

http://dx.doi.org/10.1016/j.ijmecsci.2017.07.046 Received 21 March 2017; Received in revised form 20 July 2017; Accepted 24 July 2017 Available online 12 August 2017 0020-7403/© 2017 Elsevier Ltd. All rights reserved.

<sup>\*</sup> Corresponding author at: Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong. *E-mail address:* mmmwfu@polyu.edu.hk (M.W. Fu).

and the surface layer model, Liu et al. [10] developed a new model to figure out the mechanical behavior of polycrystal. Grain boundary and grain interior are two portions in the microstructure of material, with an assumption that the mechanical behaviors of surface grain and grain interior are closely equal. The simulation by employing their model is consistent with the physical experiment. For investigation of size effect on the micro-scale amorphous polymers, Deng et al. [11] came up with an "elastic-viscoplastic" constitutive model with a consideration of rotational strain gradient. It was verified and validated by four-point microbending experiment of Poly (methyl methacrylate). In addition, Ran et al. [12] introduced the size factor into Freudenthal fracture criterion by considering surface layer model. They found that the ductile fracture happens in macroforming scenario, while it occurs with difficulty in microforming when the deformation conditions are same. In other words, the fracture strain is larger in the same deformation condition with the smaller sample size in micro-scale deformation. Gruben et al. [13] evaluated the modified Mohr-Coulomb and the extended Cockcroft-Latham and Rice-Tracey fracture criteria, which obviously explain the Lode dependence and the stress triaxiality on damage evolution. Through comparing the predicted equivalent strain at fracture initiation based on the modified and extended fracture criteria with the experimental results, they revealed that the extended Cockcroft-Latham criterion has a better prediction of the fracture strain compared to that of the extended Rice-Tracey and the modified Mohr-Coulomb criteria with a large deviation. The research, however, is more on macro-scale deformation and its validity in micro-scale deformation has not been explored. From both macro- and micro-scale deformations, the analysis and prediction of DF via consideration of surface grain, grain interior and grain boundary and their deformation behaviors in fracture formation have not yet been found based on the available literatures and this is the endeavor of this research, especially focused on micro-scale plastic deformation of materials.

From fracture formation aspect, some researchers have paid more attentions to fractographic features in ductile fracture. Li et al. [4] compared the fractographs of upsetting samples with those of tensile test samples to obtain the mesoscopic ductile fracture behavior and formation mechanism. Their observation revealed that shear-dimple ductile fracture mode exists in upsetting and tensile test samples and the stress triaxiality affects the ductile fracture mode. Shear ductile fracture occurs when the stress triaxiality is below zero. Both shear ductile fracture and void-growth ductile fracture exist together and compete with each other when the stress triaxiality is from zero to 1/3. Void-growth ductile fracture dominates when the stress triaxiality is more than 1/3. Toulfatzis et al. [14] analyzed the dimple size and distribution on fractographs of all the tested brass alloys. They found that the finest and shallowest shear dimples on the fracture surface of the CW614N leaded brass are observed, whereas the largest and deepest dimples are illustrated in the brass alloys CW511L and C27450 with absorbing the highest impact energy. Das et al. [15] employed digital image processing to determine the dimple network according to the fractographs of all the specimens. Their study indicated that there is a strong relationship among fractographic features, dimple size and density and mechanical properties. Similarly, the fractographic features on the fracture cross-section of the micro-scale specimen will be observed to analyze the fracture mode and mechanism.

In this research, a combined surface layer and grain boundary strengthening model by considering the contributions of surface grain, grain boundary and grain interior to mechanical behavior of material is developed in micro-scale plastic deformation. The physical experiments and finite element (FE) simulations of micro-tensile specimens with three different geometrical shapes and microstructural grain sizes are employed to validate the efficiency of the model. The relationship of grain size, fracture strain and stress triaxiality is thus established based on physical experiment and FE simulation by employing the newly combined constitutive model. Finally, the fractographs of the micro-tensile specimens with different grain sizes and geometrical shapes are analyzed, especially for the size and distribution of dimple in the fracture cross-section. This paper thus facilitates to advance the knowledge of deformation and ductile fracture in micro-scale deformation based working process, especially for the interaction of stress triaxiality, fracture strain and grain size and their influences on fracture formation.

#### 2. Developed constitutive model and research methodology

#### 2.1. Surface layer model

Surface and inner grains co-exist in the deformation body based on the surface layer model. Surface grains are easier to deform mainly due to few constraints compared with inner grains which have more constraints. The strength of material can be formulated below:

$$\begin{cases} \sigma = f_{surf} \sigma_{surf} + f_{inner} \sigma_{inner} \\ 1 = f_{surf} + f_{inner} \end{cases}$$
(1)

In Eq. (1)  $\sigma$  is the flow stress of material.  $\sigma_{surf}$  and  $f_{surf}$  are the flow stress and the fraction of surface grains, while  $\sigma_{inner}$  and  $f_{inner}$  are the flow stress and the fraction of inner grains, respectively.

Based on the surface layer model discussed above, a mixed constitutive model in which the flow stresses of surface and inner grains are closely equal to those of single crystal and polycrystal, respectively, was proposed by Lai et al. [8]. The single crystal model can be expressed as follows in accordance with single crystal theory and the Schmid law, also shown by Lai et al. [8] and Kim et al. [16];

$$\sigma_{\text{sig}}(\varepsilon) = \frac{\tau_{\text{R}}(\varepsilon)}{\cos\varphi\cos\lambda} = m\tau_{\text{R}}(\varepsilon) \ (m \ge 2)$$
(2)

where  $\sigma_{sig}(\epsilon)$  and  $\tau_{R}(\epsilon)$  are the flow stress of single crystal and the critical resolved shear stress, respectively.  $\varphi$  is the angle between the normal stress and the normal direction of the slip plane and  $\lambda$  is the angle between the slip direction and the normal stress. In addition, m is the orientation factor.

For the polycrystal model, the Hall–Petch relationship extended by Armstrong [17] is widely employed to represent the flow stress [8,12,16,18] in the following:

$$\sigma_{\text{poly}}(\varepsilon) = \sigma_0(\varepsilon) + \frac{k(\varepsilon)}{\sqrt{d}} = M\tau_R(\varepsilon) + \frac{k(\varepsilon)}{\sqrt{d}}$$
(3)

where  $\sigma_{\text{poly}}(\epsilon)$  is the polycrystal flow stress.  $\sigma_0(\epsilon)$  and  $k(\epsilon)$  are constants for a given strain ( $\epsilon$ ). d is the grain size and M is the orientation factor with the value of 3.06 and 2.23 for face centered cubic crystals in the Taylor and Sachs models, respectively [19].

Therefore, the mixed material model by combining Eqs. (2) and (3) proposed by Lai et al. [8] consists of two parts as follows:

$$\begin{cases} \sigma_{\text{surf}}(\varepsilon) = m\tau_{\text{R}}(\varepsilon) \\ \sigma_{\text{inner}}(\varepsilon) = M\tau_{\text{R}}(\varepsilon) + \frac{k(\varepsilon)}{\sqrt{d}} \end{cases}$$
(4)

#### 2.2. Grain boundary strengthening model

Actually, many researchers attracted by the characteristics of grain boundary have explored the material strengthening. According to Meyersm and Ashworth [20], polycrystalline aggregate is composed of grain interior and grain boundary. Hirth [21] mentioned that higher strain hardening can be generated by grain boundary compared with grain interior. The main reason is that grain boundary forbids the propagation of slip, further generating the pile-up of dislocation and strain hardening, leading to the high strength of materials in this location, also reported by Chan et al. [22]. The strength of polycrystal can be calculated as follows in the form of a composite model based on Meyersm and Ashworth [20] and Kocks [23]:

$$\begin{cases} \sigma_{\text{poly}} = f_{gb}\sigma_{gb} + f_{gi}\sigma_{gi} \\ 1 = f_{gb} + f_{gi} \end{cases}$$
(5)

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