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Void evolution in nanocrystalline metal film under uniform tensile stress

Lingling Hu [a], Jianqiu Zhou [a,b,*]

[a] School of Mechanical and Power Engineering, Nanjing University of Technology, Nanjing, Jiangsu 210009, China
[b] Department of Mechanical Engineering, Wuhan Institute of Technology, Wuhan, Hubei 430070, China

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ABSTRACT

A theoretical model to describe the nucleation and growth of voids at triple junctions of nanocrystalline metal film under uniform tensile loading is suggested. The void growth rate controlled by grain boundary diffusion under the combined influence of void surface energy, grain boundary interface energy and elastic energy stored in the solid is evaluated. Stress relaxation during uniform tension deformation is finally discussed; the effective stress relaxation distance is also calculated. The stress relaxation not only suppresses the nucleation of voids and cracks, but also influences the void growth rate.

1. Introduction

Fracture of ductile metals normally takes place by the nucleation, growth and coalescence of micron-sized voids. Of the three stages, void growth appears to be most important, since most metals deform plastically during processing or usage under this stage. Upon entering the coalescence stage, a catastrophic failure would usually occur immediately. With the experimental data discussed, the low ductility of nanocrystalline metals may be contributed to void evolution [1–3]. However, the widespread distributed void formation prior to final macroscopic fracture has few been investigated, specially void evolution in nanocrystalline metals under uniform tensile condition.

The first model of void growth was proposed by Rice and Tracey [4], who established the void growth rate and the shape changes during deformation of a spherical void embedded in an infinite matrix of a rigid-perfectly plastic solid. In the past 40 years, numerous analytical models and numerical simulations have since been carried out to explain the fundamentals of failure processes responsible for brittle behavior of most nanocrystalline metals. Analytical results by Lubarda et al. [5], Ahn et al. [6] and Meyers et al. [7] and molecular dynamics simulation by Traiviratana et al. [8] indicated that dislocation loop emission from the void surface is the primary mechanism for the void expansion. Fischer and Antretter [9] considered that the diffusion of vacancies and the mechanical driving force contribute to void growth. Inoue et al. [10] elaborated a diffusion-driven void formation model based on the mass conservation law. While Bae and Ghosh [11] developed a simple model effectively describing the void growth beyond the particle-matrix interfaces in a superplastic Al–Mg alloy. The voids after debonding, free from interface constraint grow with continued plastic deformation of the matrix with the following rates of void growth $dr/d\varepsilon$:

$$\frac{dr}{d\varepsilon} = \frac{\eta}{3}\left(r - \frac{3\gamma}{2\sigma_e}\right) \tag{1}$$

where r is the void radius, ε is the strain, σ_e is the effective stress, γ is the surface energy of void, and $\eta = d\ln v/d\varepsilon$ is the void growth rate factor, where v is the volume of a single void.

The void growth mechanisms mentioned before were mostly derived from those developed for creep deformation or superplasticity deformation [10–13]. Little knowledge has been gained in the past few decades about the void evolution in nanocrystalline metals under uniform tensile conditions. In addition, most of these reports focused on the voids nucleated from the second phase particles which existed within the materials. However, from the experimental observations, nanovoids in nanocrystalline metals usually nucleate and grow at grain boundaries (GBs) and their triple junctions during plastic deformation [14–16]. So the analysis below will focus on triple point junctions.

The conditions for void growth during uniform tensile deformation differ considerably from those assumed in the creep void growth models, but are similar to those assumed in the superplastic void growth models [11]. In the plasticity based growth model [17], the arrangement of voids was assumed as a regular array on a single grain boundary, while in this theoretical model the voids nucleate at triple junctions and one potential void nucleation site

* Corresponding author at: School of Mechanical and Power Engineering, Nanjing University of Technology, Nanjing, Jiangsu 210009, China. Tel.: +86 25 83588706; fax: +86 25 83374190.
E-mail addresses: zhouj@njut.edu.cn, yyzjqcc@sohu.com (J. Zhou).

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is isolated from other potential sites, the spacing between voids is large. All voids start to nucleate after some initial strain, exhibiting a size distribution and a gradually decreasing spacing with increasing strain. The nucleation strain for each void is also different. Furthermore, nanocrystalline materials under uniform tension experience large deformation within a much shorter time than those deforming under creep conditions. A significant grain growth is observed after the uniform tension plastic deformation, and the normal grain growth which may be due to the non-uniform GB mobility or to the local inhomogeneous stress distribution during the tensile deformation is also observed in some nanocrystalline alloys [18]. Many details of creep void growth are different from void evolution under uniform tension conditions, so it is not expected that existing models would be directly applied. Incorporation of the actual physics for nanocrystalline metals under uniform tension deformation, a corresponding novel model has been developed. In the other hand, nanocrystalline metal film is a two-dimensional structure, which is widely applied in nano-coating, packaging and nano-composites. However, mechanical behaviors and fracture characteristics of nanocrystalline metal film have few been studied through experiment and numerical simulation.

In this study, a theoretical model that describes the void evolution process in nanocrystalline metal film under uniform tensile stress, induced by grain boundary (GB) sliding through triple junctions in deformed nanocrystalline metal film is proposed. The dimple fracture process is briefly described, and the effects of surface energies, yield stress and grain size on the void growth rate are also clarified. Finally, we discuss stress relaxation during void evolution.

2. Void evolution model

2.1. Void nucleation

The fundamental mechanisms of mechanical behavior of nanocrystalline metals are difficult, because of their complex microstructures. Molecular dynamics (MD) simulations of nanocrystalline Cu by Schiøz and Jacobsen [19] found that the deformation mechanisms changed from dislocation slip to GB-mediated processes when grain size was reduced to the critical grain size d_c. Taking nanocrystalline copper for example, because the stacking fault energy of Cu is 78 mJ m^{-2} [10], the critical grain size ($d_c \approx (2/3)(Gb^2/\Gamma)$ [20]) is estimated to be approximately 100 nm. In principle, for nanocrystalline metals, grain boundary mechanism is proposed to be the dominant deformation mechanism at grain sizes <50 nm [3]. Wei et al. [21] and Gleither [22] suggested that GB diffusion along with GB sliding provided the main contribution to plastic deformation of nanocrystalline materials even at room temperature. While experiments performed on nanocrystalline Ni indicated that little dislocation storage was found at room temperature [23,24]. These indicated that deformation mechanisms not only depended on the nanocrystalline grain size but also on deformation conditions such as temperature. In this paper, the dominant deformation mechanism in nanocrystalline metal film under uniform stress deformation is assumed to be GB-accommodated mechanism. The nucleation and growth of the voids are mainly related with the GB-mediated processes, accommodating by the dislocation activities.

The main mechanisms responsible for void nucleation are listed below.

- Voids formed by dislocation emission from grain boundaries.
- Voids formed by grain-boundary sliding which leaves wedges at triple junctions. It will be discussed in detail in this paper.
- Voids formed by the action of grain-boundary sliding on the ledges.
- Voids formed by debonding along certain particle-matrix interfaces.

These nucleation mechanisms are shown in Fig. 1. The spacing of these nucleation sites is larger than grain size, determining the dimple size. The hypothetical dimple size is shown in Fig. 1(a).

In the early stages of deformation, intragranular slip is combined with unaccommodated GB sliding to facilitate void nucleation at the grain boundaries, while little dislocations are emitted from the grain boundaries under certain applied stress. Actually, when uniform tensile stress applied in nanocrystalline metal film comes up to a certain value, GB sliding commonly occurs by either local shear events or movement of GB dislocations, leading to accumulation of sessile dislocations and dipoles of wedge disclinations at and near triple junctions. Following Ref. [25], both wedge disclination dipoles and sessile dislocations storage appearing in nanocrystalline metals during GB sliding create very pronounced strain hardening. Stress concentration are likely to develop at these sites, and a void is generated to release the strain energy of the sessile GB dislocation induced by numerous acts of GB sliding at the triple junction (as shown in Fig. 1(b)). In the other hand, for identifying conditions under which voids may nucleate at triple junctions, it is necessary to consider mechanisms by which stress concentrations can be relieved. In general, stress concentration can be relieved by the faster of two processes: diffusion or dislocation. Chokshi [13] demonstrated that stress concentrations caused by grain boundary sliding were likely to be relaxed rapidly by diffusion processes not by dislocation processes.

Analysis of void evolution indicates that a stress concentration is necessary for nucleating voids [26]. The general model for stress concentrations caused by a pile-up of dislocations is shown in the following expression [13]:

$$\phi = 2\left(\frac{L_p}{b_{bg}}\right)\left(\frac{\sigma}{G}\right) \tag{2}$$

where ϕ is the stress concentration factor, b_{bg} is the magnitude of the Burgers vector of a grain boundary dislocation which is half the magnitude of the Burgers vector of a lattice dislocation, and L_p is the length of the dislocation pile-up (grain size). In general, for uniaxial tension, the value of ϕ is shown to be in the range of 1–2. When the value of ϕ is greater than a factor of ~2, the stress concentration may not be sustained substantially.

2.2. Void growth model

Several nanograins are present in the thickness direction of nanocrystalline metal film, for the ease of getting the cylindrical through voids. Uniform tension stresses below the tension yield strength of nanocrystalline metal are imposed to ensure the void formation under the condition of minimum dislocation-based plastic deformation. In this case, nanocrystalline metal film is subject to a plane state of stress in the plane perpendicular to the film thickness direction. For simplicity, let us first consider that the void keeps its cylindrical shape before void coalescence starts, and a potential void nucleation site is isolated from the other potential sites. ρ is the radius of void, R is the effective radius of void. An approximate model is described in Fig. 2(b), which is a quarter of a circular; the cylindrical void is assumed to be subject to an external uniform stress q, when $R \gg \rho$ and $\rightarrow\infty$. And grain boundaries are aligned to the radial direction with respect to the void center. In a first approximation, grain boundary phase has an elastic-perfectly plastic material behavior, and an elastic-perfectly plastic behavior is assumed with a yield stress σ_f constant in time. In this section,