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Ductile mechanisms of metals containing pre-existing nanovoids

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The void growth in monocrystalline Cu and Fe are investigated by molecular dynamics simulations to reveal the ductile mechanisms based on dislocation emission and propagation. The results show that the void growth in Cu is governed by the collective interaction of stacking faults along four (1 1 1) planes. Three dominant mechanisms of void growth in Fe are identified: (i) for small voids, nucleation of twinning boundaries; (ii) for intermediate voids, emission of shear loops; (iii) for large voids, stacking faults nucleate at the void surface and then degenerate into shear loops. The slip-twinning transition rate of Fe at room temperature calculated according to Zerrili-Armstrong model is in the range measured by our atomistic simulations. Vacancy generation which promotes void growth results from the intersection of more than two stacking faults in Cu, while in Fe it is related to the movement of screw dislocations. An analytical model based on nudged elastic band calculation is developed to include the strain rate dependence of the nanovoid-incorporated yielding. This new model demonstrates that the critical stress for dislocation emission will decrease with increasing strain rate and dislocation core width. For both metals, the dislocation density has been calculated to elucidate the plastic hardening coupled with void growth. This work sheds new lights in exploring the atomistic origins of the void size and strain rate dependent mechanisms associated with dislocation activities close to void surface.

1. Introduction

It has been commonly agreed that the ductile fracture of metals is closely related to the nucleation, growth and coalescence of voids. For instance, the void nucleation can be initiated by second phase inclusions, the sliding of grain boundaries and spallation during the process of shock loading. In order to envision the physics beneath the ductility, many mechanisms have been proposed. At the continuum scale, a model was proposed in [1], where they considered a single void in an infinite solid, and solved the rate of void growth. However, an obvious disadvantage of the Rice and Tracey (RT) model is the neglect of the interactions between voids. Another model, initially proposed in [2] and later modified in [3–6], which is well known as GTN model, considered a porous medium behaving as a continuous and homogeneous continuum. Besides, the influences of initial parameters on the void evolution, such as strain rate [7–10], initial void volume fraction (vvf) and stress triaxiality [11–14], have been studied. Void coalescence is the final stage of ductile fracture. A plastic limit model for coalescence based on the competition between localized and homogeneous deformation was proposed in [15–17]. Finite element calculations of void coalescence were performed in [18] and a critical parameter named the intervoid ligament distance (ILD) was proposed. Experiments [19–22] have revealed the effect of coalescence on materials failure due to void impingement. The so called complete Gurson model [23–25] was proposed to account both void growth and coalescence, which is accurate for both non-hardening and hardening materials. A detailed review on the ductile behavior of voids can be found in [26].

A considerable number of works have contributed to a better understanding of the microscopic mechanism of void evolution. The void growth mechanism was developed under the consideration of vacancy condensation in [12]. This model can accurately predict the time required to nucleate a void in front of a crack tip, if the dislocation pipe diffusion is considered. However, it has been pointed out that this mechanism cannot work under high strain rate loading. For example, the time required for a void growing to a size of $\sim$0.1 μm is 10^5 s even at a temperature nearly 2000 K. Thus, this vacancy diffusion mechanism is not an appropriate model for the conventional plastic deformation as discussed in [27]. In high strain rate shock loading experiments, this mechanism certainly failed to depict critical failure such as spallation. Inspired by these pioneer works and the Ashby mechanism for

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the generation of geometrically necessary dislocations (GND) [28], it was believed that the void growth is promoted by a continuous emission of dislocation loops attached to the void surface [29]. It should be noted that, the dislocation based deformation mechanisms have also been independently proposed in [30,31].

Molecular dynamics (MD) allows us to directly observe the motion of dislocations, and enrich our knowledge about materials at nanoscale. One of the first MD simulations of void evolution was performed in [32], and designed to model spallation caused by tensile release waves in shock experiments. The stress-strain response and the effect of triaxiality on void growth and coalescence were investigated in [33–35], and it was found that the stress triaxiality plays a significant role in the evolution of void shape at the early stages after plastic yield. It should be noted that these works do not involve any analysis of the motion of dislocation. This situation has changed since the dislocation-based model was proposed in [29]. The first remarkable verification of this mechanism was inaugurated in [36], where the dislocation activity of a bulk Cu with a spherical void in the center was studied under uniaxial tension. Bulatov et al. [37] made an important comment on the impossibility of void volume change caused by the motion of detached shear loop. This question was answered by introducing the concept of cooperative shear slip [38]. The effect of loading orientation and grain boundaries on the evolution of voids was thoroughly examined in [39,40], and it was found that the loop configuration depends on the loading direction. Although these studies have improved the understanding of grain boundary effect on ductile fracture, it is still unclear how grain boundaries influence the spallation of materials under dynamic loading [41,42]. Benefiting from the work in [29,36,39,40], a new model to calculate the critical stress required to generate a shear loop on the void surface was proposed in [43]. In this model, they observed the creation of the surface step which was not considered in [29] would result in a different estimate of the critical stress. Recently, a new continuum model [44] was developed based on the multiplication of dislocations.

It is always intriguing to discuss the relation between nanoscale simulations and continuum theories. The mechanism underlying the plastic deformation of an Al crystal with a nanovoid was revealed by using the quasicontinuum method [45,46]. The MD studies focused on the stress-strain response and the evolution of vvf were performed in [47,48], and compared with continuum theory. These results proved that the Gurson model [2] fails to capture the size dependence of the critical yield stress in the interpretation of such a nanoscale phenomenon. A full MD examination of the Lubarda-Meyers model [29] was performed and compared with the Cocks-Ashby model [9] for the evolution of vvf [49]. Because the yield stress is a key parameter in the continuum models of ductile fracture, it is necessary to have a good knowledge of the dislocation evolution. In the MD simulations performed in [47,50], it was found that the interaction between voids is accomplished by the dislocation loops emitted from the void surface. Besides, the annihilation and formation of dislocation densities can lead to significant differences in void interaction behavior according to [51].

The majority of previous studies have focused on two aspects, i.e., the void size effect on deformation behavior and how to bridge the gap between nanoscale simulation and continuum models. However, as another important parameter influencing the ductile mechanisms, strain rate should not be ignored. Here we report a full examination of both void size and strain rate effects by atomistic simulations. Besides, only a few works have been done to explore the interaction between voids mediated by the dislocation evolution. Thus, we will also calculate the dislocation density of nanovoided metals. The goals of the present study can be summarized as: (1) study the effect of strain rate and void size, on the dislocation behaviors during plastic deformation; (2) provide a standard method to predict the critical yield stress of nanovoided metal by considering the effect of strain rate; (3) quantitatively analyze the plastic activity based on measurements of the dislocation density. The sections are organized as follows. In Section 2, the computational settings are described in details. The results of the void size effect on dislocation evolution mechanisms are presented in Sections 3.1 and 3.3. In Sections 3.2 and 3.4, the strain rate effect is studied. An analytical model based on classic nucleation theory is proposed in Section 3.5 and in Section 3.6 the dislocation density is calculated using the dislocation extraction algorithm.

2. Computational details

Molecular dynamics (MD) simulations were carried out using LAMMPS [52] with a widely used embedded atom method (EAM) potential for fcc Cu [53] and a Finnis-Sinclair potential [54] for bcc Fe. In order to investigate the void size dependence of plastic deformation, we designed cubic boxes with different void radius, as shown in Table 1. The void is placed at the center of the cube. The *xyz* coordinate axes are along $\langle 100 \rangle$ directions. Periodic boundary conditions are applied along all three dimensions. For the deformation analysis, the simulation boxes are relaxed at 300 K for 20 ps in the isothermal-isobaric (NPT) ensemble. The Velocity Verlet algorithm is employed to integrate the equation of motion with a timestep of 1 fs. During tensile loading, we use the microcanonical (NVE) ensemble to eliminate the influence of external heat sources and capture the temperature evolution in order to calculate the density of mobile dislocations. Except the investigations of strain rate dependence, all the other simulations are performed with a constant strain rate $\dot{\varepsilon} = 10^8\ \mathrm{s}^{-1}$. The common neighbor analysis (CNA) technique [55,56] is employed to filter the defected atoms generated during loading process, and the centrosymmetry parameter (CSP) [57] is calculated to render the output images. The newly developed dislocation extraction algorithm (DXA) [58] enables us to make quantitative analysis of dislocation density. To detect the vacancy in bcc lattice, we recompiled the library of DXA and add a new structure pattern. We use Ovito [59] and AtomViewer [60,61] to visualize the dislocation structures.

3. Results and discussions

In this part, we illustrate the effect of void size and strain rate on dislocation emission at void surface. To the best of our knowledge, previous models [29,43] can accurately describe the void size dependence of yield stress, but no analytical model is proposed to depict the rate dependence. Based on the calculation of energy difference during the process of shear loop nucleation, we develop a new model which is capable of extending the MD results to the laboratory strain rate situation. As an important quantity to measure the void interaction, dislocation density is calculated using the DXA algorithm.

3.1. Ductile deformation in Cu – void size effect

The sequence of dislocation nucleation, growth and multiplication in a $d = 16a_0$ Cu specimen under uniaxial tension is shown in Fig. 1. In Fig. 1(a), we can see that once the stress reaches the elastic limit, "clusters" are activated and randomly distributed in the simulation box before the nucleation of dislocations from the void surface. In Fig. 1(b), it is found that dislocation loops are emitted along two adjacent slip planes. Then, collective multiplication of dislocations will promote continuous growth of the void volume. In Fig. 1(c) and (d), the stacking faults activated in $(\bar{1}\,\bar{1}\,1)$, $(1\,1\,1)$ and $(1\,\bar{1}\,\bar{1})$ planes form a spade-like dislocation microstructure. In