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Molecular dynamics simulation of the influence of elliptical void interaction on the tensile behavior of aluminum

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ABSTRACT

The effect of void interaction on the damage progression in aluminum under uniaxial tension is studied via molecular dynamics (MD) method. MD geometries containing two adjacent elliptical voids are created with different void shape combination and intervoid ligament distance (ILD). The dislocation emission and development, stress–strain relation, porosity accumulation, void shape evolution and ILD shrinkage are monitored during loading process. The critical stress required by the voids to trigger the dislocation emission is in line with the prediction of the Lubarda model under the uniaxial tension case. Our results indicate that the onset strain of dislocation emission is mainly subject to the void shape. The void shape combination is found more influential than the ILD on the stress response and the porosity accumulation.

1. Introduction

The initiation and evolution of small voids limit the formability and ductility of aluminum and its alloys. These voids grow and coalesce during the continued applied loading, causing localized coalescence and fracture. A famous constitutive model was proposed by Gurson [1] to account for the void's role in characterizing material damage. Tvergaard [2] introduced adjustment parameters to further calibrate the Gurson relation based on micromechanical studies on periodically distributed voids. So far, these models or their variants have been widely incorporated in finite element (FE) simulations and analytical calculations. Most of the constitutive models for porous metals are derived by the unit cell modeling. However, the voids in a real engineering material are not likely to be uniformly distributed. In order to capture the softening response of the porous metals with higher accuracy, it is physically necessary to characterize the heterogeneity of the void distribution. Indeed, heuristic study on the effect of void interacting in porous metals has been carried out via the FE method or the analytical approach by many researchers. Ohno and Hutchinson [3] concluded from their model, which embedding an excess of voids within a disk-shaped cluster with a uniform background distribution to an elastic–plastic solid, that non-uniform distribution of the voids lowers the ductility. Later, this conclusion was supported by Becker [4], who used a distribution of initial porosity from experiments to perform the finite element simulation. Magnusen et al. [5] examined the specimen with random or uniform distributions of macroscopic holes and developed an algorithm in modeling. Benson [6] applied an Eulerian finite element program to study the dynamic response of OFHC copper and 4340 steel by assuming an arbitrary random distribution of six voids with fixed total porosity. Later, Benson [7] studied the void clustering effect by modeling a discrete set of randomly distributed clusters. He found that the ultimate stress is a constant with the changing fracture strain and with the void cluster diameter. Horstemeyer et al. [8] employed the micromechanical FE method to quantify the coalescence effect based on temperature and different spatial arrangement of voids. He also proposed a critical ILD to define void coalescence. Chen et al. [9,10] applied the FE-damage percolation model to study the damage evolution in the forming of aluminum alloy sheets. This damage percolation model adopted elliptical void shapes and employed measured particle distribution to characterize the void cluster initiated by second phase particles. Toi and Kang [11] carried out a 2D mesoscale simulation to analyze the elasticity, yield stress and void-linking fracture via meshless method. Bilger et al. [12] paid attention to the specific role of the porosity fluctuations inside the representative volume element. Their results indicated the porosity fluctuations can have a strong effect on the overall yield surface of porous materials. Gărăjeu and Suquet [13] focused on the influence of small fluctuations of porosity on the effective properties of porous materials. They concluded that deviations of uniform distribution result in weakening the macroscopic load carrying capacity of the porous materials. The

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experimental research [14] using drilled-hole samples revealed different failure and strain pattern depending on the configuration of the microvoids and also highlighted the importance of void spacing and void orientation. Bandstra and Koss [15] examined the sensitivity of void growth and coalescence to the intervoid spacing, strain hardening and multiaxial stress state. They concluded that the growth of voids within the cluster is accelerated. The work of the above researchers demonstrates the important role of the void interaction in the damage progression ranging from the microscale to the macroscale.

As for nanovoids, evidence suggests that dislocation-void interaction plays an important role in the void evolution in metals [16–23]. Lubarda [17] extended his early work [16] to a more generalized dislocation-void interaction model under combined loading. The minimum critical stress is physically obtained by minimizing the critical stress with respect to the two angular variables. Both the dislocation emission angle and critical stress predicted in [16] were supported by MD simulations [22–25]. So far, the void growth and coalescence mechanisms in face-centered cubic (FCC) metals have been widely studied by the MD simulation. Potirniche et al. [26] employed the MD method to study growth and coalescence of circular nanovoids in single crystal nickel. Their results reflected the size-scale dependence of the nanovoids. Traiviratana et al. [24] performed the MD simulation in monocrystalline and bicrystalline copper. The emission of dislocation is confirmed to be the primary mechanism of void growth. Bringa et al. [25] applied the MD method to investigate the effect of loading orientation and nanocrystalline in FCC copper. Marian et al. [22] used the quasi-continuum method to study the void expansion in FCC aluminum and indicated that dislocation emission is the primary mechanism. However, the investigation of the role of void interaction including the intervoid spacing and void shape combination has not been reported. Therefore, efforts are made here to elucidate and examine the role of void interaction in the material response of the FCC aluminum.

The void interaction simulation regards the voids of elliptical shape. The elliptical void, as a generalized treatment of the initial void geometry, highlights the role of the void shape. It has been acknowledged that the initial void shape has considerable influence on void growth, coalescence and material softening [27–30]. Some detailed studies regarding the effect of initial void shape via FE method have been carried out in [29,30,27]. They concluded that the effect of void shape can be substantial on the porosity evolution and influential on the stress–strain relation. Indeed, some analytical models such as the Gologanu–Leblond–Devaux (GLD) model [31] model or its more sophisticated variants [28,32,33] have already included the influence of void shape phenomenologically. However, in MD simulations, most authors adopted circular or spherical void shape as a geometric simplification. The pertinent intervoid geometries [34] are depicted in Fig. 1. For the empirical approach, void coalescence occurs through shear band development between the neighboring elliptical voids when the ILD satisfies the criterion with regards to the void geometry [34]. As illustrated in Fig. 2, the critical ILD is larger than zero for the empirical criterion as a simplification to the physical problem. However, the void coalescence process, as observed both in MD simulations and experiments, is likely to be a continued process. Therefore, a task of paper is to investigate the continued process of void coalescence under the interaction of elliptical void via MD simulation.

In this work, a 3D simulation box with a thin z-direction thickness is employed. As shown in Fig. 3, it has doubled length in y-direction based on the fact that void coalescence occurs perpendicular to the uniaxial loading direction. The simulation box can be viewed as the combination of the upper and lower square unit cells. The resulted void distribution in the simulation box is no longer uniform. A benefit of this "2D" simulation geometry is that

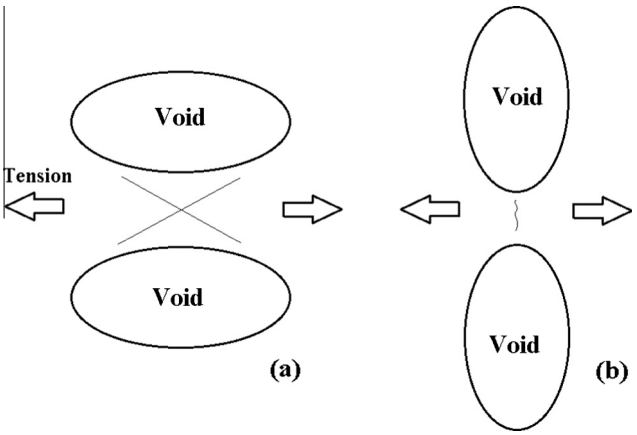

Fig. 1. Schematic of idealized void interaction geometry reproduced from [34]: (a) oblate–oblate combination; (b) prolate–prolate combination.

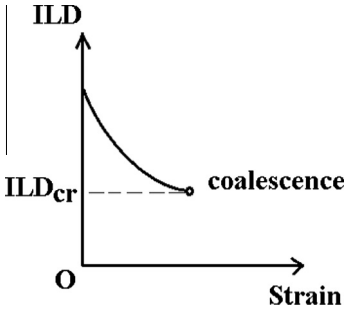

Fig. 2. Schematic of the empirical criterion for void coalescence (the critical ILD is larger than zero).

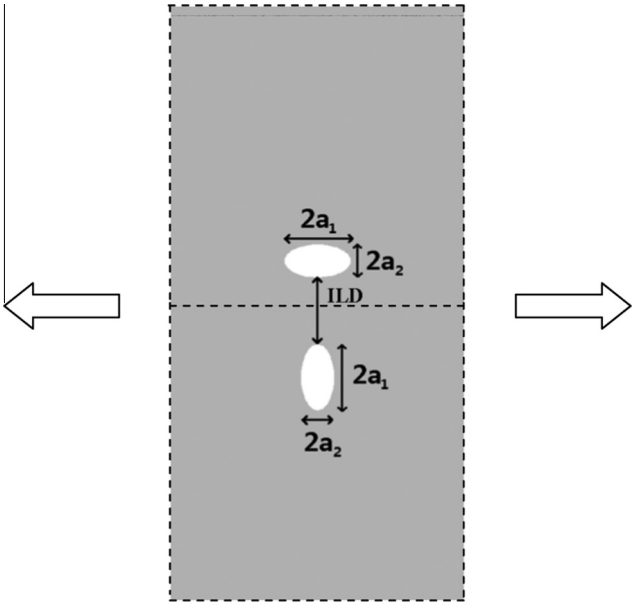

Fig. 3. Simulation geometry containing two non-uniformly distributed elliptical voids (periodicity are applied on all the three dimensions).

it allows us to have a clear view of the material transport in the high strain regime when the primary growth of the voids prevails. Chang et al. [35] suggested that the yield stress simulated by MD in 2D is very close to that in 3D at 0 K. Nevertheless, the extension toward a cubic 3D simulation geometry would be helpful in that it provides spacing space in the third direction for the motion of