**Rare Metal Materials and Engineering**
Volume 43, Issue 7, July 2014
Online English edition of the Chinese language journal

**Cite this article as:** Rare Metal Materials and Engineering, 2014, 43(7): 1571-1576.

ARTICLE

# Void Shape Effects on Void Growth and Slip Systems Activity in Single Crystals

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**Abstract:** Cast void shape effects on void growth and slip system activity in single crystals were studied using crystal plasticity under various orientations of the crystalline lattice. A 3D unit cell with ellipsoidal void was set up using three-dimensional 12 potentially active slip systems; the spherical shape of void which is a special case of ellipsoid was also included. The numerical results show that the initial texture orientation, the ellipsoidal coordinate, the load coordinate system and the shape of void have a competitive effect on the evolution of voids. For triaxial tension conditions, the void fraction increase under the applied load is strongly dependent on the shape of void and the crystallographic orientation with respect to the load axis, as well as the activities on all the slip systems. When the symmetry of the unit cell is broken, the void experiences a rotation in spite of the load applied along <001> and <011> orientations with symmetry of the slip systems. An interesting feature is that, even in the case of anisotropic crystalline matrix materials, the overall effect of plastic anisotropy on damage evolution is diminished during non-spherical void growth.

**Key words:** void growth; shape effect; single crystal; orthotropic; crystalline orientation; slip system

The ductile fracture occurring through the nucleation, growth and coalescence of voids, is a primary mode of material failure, so it is important to predict the condition of void growth and coalescence when a material is subjected to large plastic deformation.

Analytical and computational investigations[1-12] were conducted to characterize and understand void growth and flow localization. Essentially all of these analytical and computational investigations were based on phenomenological inelastic constitutive relations such as $J_2$ plasticity or Gurson's[4] constitutive formulation, but there still exists much deficiency in this model [13-15]. Crystal plasticity model is a hot topic in the damage mechanics area, and most of the microstructures, such as inclusions, grain boundary and crystallographic slip can be taken into account. Most recently, based on this theory, the interrelated effects of porosity, initial void size, hydrostatic stress, geometrical softening, void distribution, and work-hardening rate on void growth, failure paths, ligament damage and coalescence behavior in face centre cubic (fcc) have been investigated [16-20], which were implemented with the 2D circle-void unit cell or 3D model with spherical voids. Actually the voids which nucleate from second-phase particles have highly irregular shape, so it is necessary to address 3D model with non-spherical voids, and computational evaluations of this nature are valuable because they provide an approach to quantitatively assess micro-macro relations, and to illustrate the relation of void growth with void shape directly.

In this paper, the rate-dependent crystal plasticity theory[12] is applied to investigate void growth in fcc single crystals. To illustrate the behavior of void growth for different shapes, the 3D unit cell including an ellipsoidal void was considered here. By changing the ratio of three axes for ellipsoid, three voids with different shapes were investigated.

## 1 Geometrical and Boundary Condition

### 1.1 Unit cell model

The ellipsoid was used to describe the shape of void (Fig.1). Assuming that the void nucleation has already occurred, a single ellipsoidal void was embedded in the unit

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Received date: July 15, 2013

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cell which is a cubic with one side length $L$, as shown in Fig.2. Such a unit cell model which is a representative volume element of uniformly distributed voids in a medium can effectively represent the interaction effects between voids[16,17]. The finite element meshes used in the simulations are presented in Fig.2.

In the case of the one-void unit cell, the initial void volume fraction $f_0$ is as follows:

$$f_0 = \frac{4\pi}{3}\frac{r_1 r_2 r_3}{L^3} \tag{1}$$

Where $r_1$, $r_2$, $r_3$ are the half-axis length of three axes ellipsoidal sphere respectively. $f$ is the void volume fraction calculated during solution and $R$ is the normalized void volume fraction

$$R = f / f_0 \tag{2}$$

### 1.2 Boundary condition

For all orientation, all unit cells were subjected to the same triaxial strain field by applying a proportional displacement along the three axes $x$, $y$ and $z$. The applied displacement in the $x$ direction is $\delta$, while in the $y$ and $z$ direction, it is $a\delta$ and $b\delta$, respectively, as shown in Fig.3. Similar boundary conditions were also considered by Shu[21].

### 1.3 Coordinate systems

The coordinate systems used in the simulations are presented in Fig.3. The $x$-$y$-$z$ represents the load coordinate system, and it is the coordinate system where unit cell edge is located; <001>-<010>-<100> is the material coordinate system, where $\alpha_0$, $\beta_0$, $\gamma_0$ are the transform angles between material coordinate system and load coordinate system; $R_1$-$R_2$-$R_3$ is the coordinate system where the three axis of ellipsoidal void are located, while $\alpha$, $\beta$ and $\gamma$ are the transform angles between the ellipsoidal coordinate system and the load coordinate system.

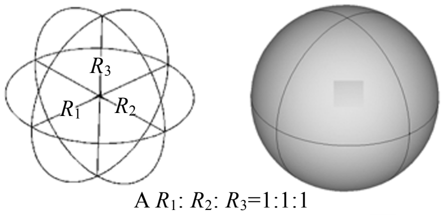
## 2 Results and Discussion

In this section, the results from the finite element simulations relating to the ellipsoidal void effects on the void growth are analyzed. The strain controlled boundary conditions were employed in this study and the load triaxiality factor $a$=$b$=–0.235, as shown in Fig.3. The initial void volume fraction is $f_0$=0.01 and $L$=50 μm. The interrelated combination of crystal orientations, ellipsoidal shape and ellipsoid orientations for the analysis and corresponding symbols in this study are listed in Table 1.

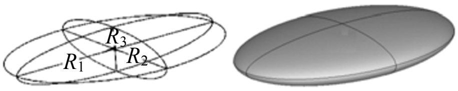
### 2.1 Void growth

#### 2.1.1 Void growth in <001> crystal orientation

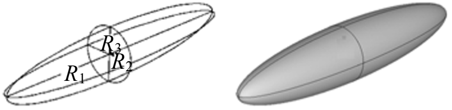
Fig.4 indicates that in the case of A-1 the peak normalized void volume fraction reaches 1.059 for the corresponding $\varepsilon_x$=0.1, while those of for B-1, B-2, B-3 and B-4 are 1.047 1.040 1.359 and 1.309, respectively. As shown in Fig.4, the growth rate of A-1 is slow, which is consistent with the previous result [17]. A more rapid increase occurs in the case of B-3 and B-4. It's worth noting that in the case of B-1 and B-2, a lower increase occurs than A-1, but the difference is minor.



A $R_1$: $R_2$: $R_3$=1:1:1



B $R_1$: $R_2$: $R_3$=5:5:3



C $R_1$: $R_2$: $R_3$=5:3:3

Fig.1 Geometrical of ellipsoidal void

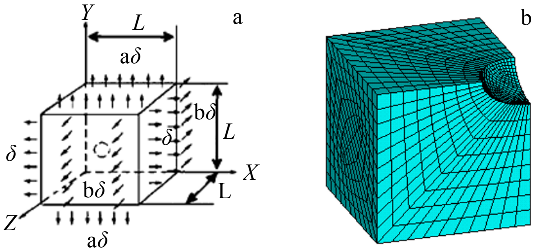


Fig.2 Boundary conditions (a) and finite element mesh (b)

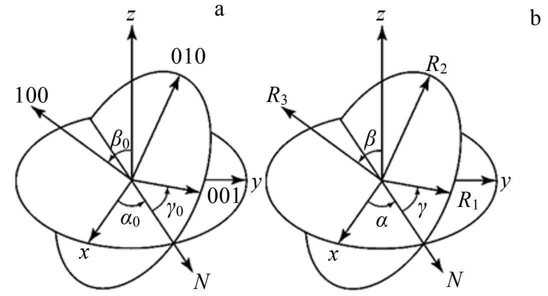


Fig.3 Material coordinate (a) and ellipsoidal coordinate (b) vs. load coordinate system

Fig.5 indicates that corresponding to C-1, C-2, C-3 and C-4, the peak normalized void volume fractions reach 1.121 1.113 1.345 and 1.233, respectively, for the corresponding $\varepsilon_x$=0.1. Compared with A-1, the void tends to grow easily in the cases of C-1 and C-2, especially in the cases of C-3 and C-4.

#### 2.1.2 Void growth in <011> crystal orientation

Ellipsoidal shape B shows a relatively similar distribution between <011> and <001> crystal orientation, as shown in Fig.4 and Fig.6. In Fig.6, the peak normalized void volume fractions of shapes A-2, B-5, B-6, B-7, and B-8 reach 1.336 1.056 1.036 1.438 and 1.379, respectively,