Nanovoid deformation in aluminum under simple shear

Jaime Marian *, Jaroslaw Knap, Michael Ortiz

Division of Engineering and Applied Science, California Institute of Technology, Pasadena, CA 91125, United States

Received 2 February 2005; received in revised form 19 February 2005; accepted 22 February 2005
Available online 9 April 2005

Abstract

We analyze the mechanisms underlying the deformation of a nanovoid in an Al crystal subjected to cyclic shear deformation using numerical simulations. Boundary and cell-size effects have been minimized by means of the quasicontinuum method. The deformation of the void entails a noticeable reduction in volume. During the loading phase, our analysis reveals several stages of stress buildup separated by yield points. The main mechanisms underlying the deformation of the crystal are: glide of primary and secondary partial dislocation loops with mixed edge-screw character; intersection of primary and secondary loops to form jogs and junctions; cross-slip; and dislocation multiplication and annihilation. Cross-slip occurs by the Fleischer mechanism and not by the more commonly assumed Friedel–Escaig mechanism. During unloading, most of the dislocation population and void volume reduction is recovered by re-absorption of dislocation loops and annihilation mediated by cross slip. However, a residual dislocation density remains around the void at the end of the unloading process.
© 2005 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

Keywords: Quasicontinuum; Aluminum; Dislocations; Cross-slip; Ductile fracture

1. Introduction

The formation of spall planes in shocked metals is believed to be the result of processes of void nucleation, growth and coalescence (cf., e.g. [1]). Recent experimental data suggest that the material response within a strong shock is essentially volumetric [2] and, consequently, most studies of void dynamics to date have concerned void expansion under hydrostatic tensile pressure (e.g. [3–8]). The behavior of voids under general states of stress and deformation remains comparatively much less well understood. This is a particularly glaring gap in our knowledge since void growth does in many cases of interest involve a certain combination of expansion and shear. Instances of this mixed-mode void growth include the classical cup-cone failure of uniaxial tension specimens [9]; void formation leading to ductile rupture in shear bands [10]. Moreover, nanoscale studies of void dynamics are often intended as a step towards the formulation of multiscale models of shocked metals. In this particular framework, a complete quantitative understanding of void dynamics under general load and deformation paths, including combinations of expansion and shear, rotating principal directions of stress and deformation, and loading/unloading cycles, is of essence.

As a step in that direction, in this paper we focus on the shear response of Al single crystals containing nanosized voids. At that lengthscale, molecular dynamics (MD) suggests itself as a natural analysis tool [4–7]. MD studies have revealed, among other useful insights, that nanovoids exceeding a pressure and temperature-dependent critical size grow by the emission of dislocations and by coalescence with neighboring voids. MD is particularly well-suited to the study of void growth at very high strain rates, often greatly in excess of those
attained experimentally. In addition, reliance on periodic boundary conditions limits the range of elapsed times which can be examined by MD and may introduce undesirable artifacts. Continuum estimates [3] suggest that dynamic effects are negligible for small voids at moderate-to-high strain rates. These considerations point to the need to complement MD studies with detailed analyses of the equilibrium energy landscape and transition paths accessible to deforming nanovoids. The technique that we use in order to carry out such an analysis is the quasicontinuum (QC) method [11,12].

We specifically consider the deformation of a 5.2-nm nanovoid in Al (modeled using a well-tested potential [13]) under prescribed macroscopic simple shear deformations in the range of 0–20%. The principal questions addressed in this study concern: (i) the mechanisms of deformation in the vicinity of the nanovoid during loading and unloading; (ii) the resulting microstructures; and (iii) the determination of macroscopic behavior such as the change in volume and shape of the void, the shear stress–strain curve and the extent of plastic work and hysteresis. Following a brief description of the method of analysis and the boundary value problem in Section 2, in Section 3 we proceed to report in detail the complex sequence of mechanisms by which the void distorts and changes its volume under the action of the prescribed macroscopic shear. Some of the predicted mechanisms are unexpected. For instance, we find that, in Al and under the conditions of this analysis, cross-slip occurs according to the Fleischer mechanism [14] and not by the commonly assumed Friedel–Escaig mechanism [15,16]. The macroscopic behavior of the sample is found to contain several stages of deformation, punctuated by yield points characterized by abrupt changes in the operating deformation mechanism, rapid microstructural changes and sudden stress drops.

2. Calculation preliminaries

QC is a method for systematically coarse-graining lattice statics models [11,12]. The method starts with the complete atomistic system and reduces the configuration space of the crystal through judicious application of finite-element-based kinematic constraints. In order to avoid full lattice sums, cluster summation rules are used. By virtue of these rules, only atoms in small clusters surrounding the representative atoms need be visited in computing the effective out-of-balance forces. Finally, the selection of representative atoms is performed adaptively based on a local strain measure and longest-edge tetrahedral bisection. The tolerances governing the adaption process are set such that full atomistic resolution is attained in the presence of dislocations. The QC method uses empirical potentials directly as the sole description of material behavior and contains fully atomistic lattice statics and continuum elasticity as special limits. As in conventional continuum mechanics, QC permits the direct simulation of systems controlled through the application of remote boundary conditions, a feature that is particularly useful in simulating dilute distributions of nanovoids. QC simultaneously provides atomistic resolution at defect cores without the stringent size limitations of direct atomistics. Details of the implementation of QC used in the present study and an analysis of the accuracy and convergence of the method may be found in [17].

We specifically consider the shear response of Al single crystal samples containing nano-sized voids and subjected to a macroscopic (homogeneous) deformation gradient of the form

$$\mathbf{F}_h = \mathbf{I} + \gamma \mathbf{l} \otimes \mathbf{m},$$

(1)

where $\mathbf{I}$ is the identity tensor, $\mathbf{l}$ and $\mathbf{m}$ are two orthogonal unit vectors ([100] and [010], in our case) and $\gamma$ is the prescribed macroscopic shear strain. We increase $\gamma$ gradually from 0% to 20% by 1% increments. A principal outcome of the calculations is the plastic work budget and degree of hysteresis associated with nanovoid growth. In order to ascertain these aspects of the macroscopic behavior of the material we proceed to calculate the recovery curve resulting from the unloading and reverse-loading of the sample back to its initial macroscopic configuration. In the simulations, we induce this unloading by reducing $\gamma$ to zero following the attainment of its maximum prescribed value of 20%.

At each loading step, a new stable equilibrium configuration is obtained by means of the Polak–Ribiere variant of the conjugate gradient algorithm [18]. The computational mesh is then adapted so as to adequately resolve the fine features of the solution. The precise adaption indicator employed in the calculations reported here is as follows. Suppose that $\mathbf{F}$ is the local deformation gradient of a tetrahedron $K$ in the computational mesh. The departure of that local deformation $\mathbf{F}$ from the macroscopic deformation $\mathbf{F}_h$ is $\mathbf{F}_r = \mathbf{F} \mathbf{F}_h^{-1}$. We flag $K$ for refinement when the norm of the second invariant of the corresponding Lagrangian strain $\mathbf{E} = \frac{1}{2} (\mathbf{F} \mathbf{F}^T - \mathbf{I})$ exceeds a pre-specified tolerance. As mentioned before, this tolerance is chosen such as to ensure full atomistic resolution well in advance of the passage of dislocations.

The computational cell used in simulations is a 174-nm cube of face-centered cubic (fcc) Ercolessi–Adams Al [13] containing $432 a_0 \times 432 a_0 \times 432 a_0$ unit cells ($a_0 = 4.032$ Å), or a total of $3.2 \times 10^6$ atoms. The cell is oriented along the cubic lattice directions. An equiaxed 5.2-nm void is initially introduced at the center of the cell. The initial triangulation of the cube is tailored to the problem geometry. In particular, full atomistic resolution is introduced in a $16a_0 \times 16a_0 \times 16a_0$ region.
around the void from the outset. Away from this region, the triangulation is gradually coarsened. The resulting initial number of nodes, or representative atoms, in the mesh is 31,933, which represents a four-orders of magnitude reduction in problem size.

In order to reliably identify the defects in the deformed crystal we employ the centro-symmetry deviation parameter [19]. For a partial dislocation core atom in Al the deviation parameter is 2.1 Å², between 5 and 20 Å² for a stacking fault, and 24.4 Å² for a \{111\} free surface. In all subsequent dislocation structure plots, atoms are colored according to the relative magnitude of their centro-symmetry deviation parameter with blue and red corresponding to free surfaces and partial dislocation cores, respectively, while atoms belonging to stacking faults are identified by means of an orange-to-yellow color gradation. Once the dislocation lines are identified, the Burgers vectors can be readily determined by performing a Burgers circuit around the dislocation core. Finally, the edge and screw components of the dislocation can be resolved by resorting to the following pair of simple expressions:

\[
\mathbf{b}_e = (\mathbf{b} \cdot \xi) \cdot \xi, \\
\mathbf{b}_s = \xi \times (\mathbf{b} \times \xi),
\]

where \(\mathbf{b}\) is the total Burgers vector and \(\xi\) is a unit vector tangent to the dislocation line.

3. Results

3.1. Stress buildup phase

The computed shear stress vs. shear angle curve \((\tau, \theta)\) is plotted in Fig. 1. The shear stress \(\tau\) is calculated directly from the external tractions acting on the boundary of the computational cell. We define the shear angle as \(\theta = \tan^{-1} \gamma\). Both the loading, \(\tau_l\), and the recovery, \(\tau_r\), curves are shown in Fig. 1. Three main stages of rapid shear stress buildup punctuated by yield points are clearly discernible in the \((\tau, \theta)\) curve in Fig. 1: (i) an initial elastic stage up to the first yield point at \(\theta = 6.9^\circ\), characterized by the elastic deformation of the void without any dislocation activity; (ii) a second stage of stress increase up to a second yield point at \(\theta = 9.1^\circ\), characterized by the formation of pairs of dissociated perfect dislocations nucleated on the planes where the resolved shear stress (RSS) is maximum; and (iii) a third stage of hardening characterized by the nucleation and growth of shear loops and their interactions with the pre-existing dislocations. We refer to the various stages of deformation during the loading phase as stages I, II, and III, respectively, for ease of reference, and we proceed to describe the deformation mechanisms underlying these stages. Subsequently, the stress recovery phase is likewise discussed.

Stage I is a purely elastic regime, in which the only appreciable effect is the growth of the atomistic-resolution region around the void as driven by the adaption criterion. The first dislocation structures emerge immediately following the first yield point at a shear stress of 4.3 GPa, corresponding to a shear angle of \(\theta = 6.9^\circ\), which thus may be regarded as the critical shear stress for the inception of plastic deformation. The dislocation structures that form immediately after the first yield point are shown in Fig. 2. Notably, these dislocations are vacancy in nature, i.e., net mass transport occurs from the matrix towards the void. The maximum RSS occurs on two equivalent \{111\} planes located at \(\pm45^\circ\) with respect to the void axes. These primary planes serve as nucleation sites for four (two at \(+45^\circ\) and two at \(-45^\circ\)) independent leading Shockley partials. Fig. 3 shows the shear component of the displacement field superposed on the adapted triangulation at the critical shear angle of \(\theta = 6.9^\circ\). As expected, the displacement field is symmetric about the origin and is accurately resolved by the adapted mesh, which develops lobes of atomic-resolution extending at 45° to the principal cubic lattice directions and contains 133,877 nodes.

Stage II is characterized by pure glide of partial dislocations on primary slip systems. Moreover, aided by both the internal stresses and the relatively high stacking fault energy of Al, the trailing partials are able to detach from the surface of the void giving rise to a set of dissociated perfect \(\frac{1}{2} \{110\}\) dislocations. These dislocations...
are highly mobile and rapidly glide away from the void. As noted above, the dislocations are vacancy in character and are nucleated on planes that share a common \( \langle 110 \rangle \) direction coincident with their line of intersection. By virtue of this geometry, after certain initial easy glide the leading partials converge on that \( \langle 110 \rangle \) line at some distance from the void, thus creating Lomer–Cottrell locks. This reaction is consistent with the set of geometrically-possible dislocation interactions derived by Hirth [20]. Once formed, these locks temporarily obstruct further glide and shut off activity on the primary slip planes, causing a marked stress rise. When the resulting RSS on secondary slip planes reaches a critical value, new dislocation structures in the form of shear loops emerge from the void surface. This burst of dislocation emission occurs at an applied stress of 9.1 GPa, corresponding to a shear angle \( \theta = 9.1^\circ \), and results in a marked shear stress drop that signals the onset of stage III (Fig. 1). Fig. 4 shows the secondary dislocations in addition to the Lomer–Cottrell locks originated at the end of stage II. The secondary loops are highly mobile and glide easily in response to small increments of the applied stress.

Upon continued loading, secondary partial dislocation loops with mixed edge-screw character bow out away from the void. Edge segments are seen to have higher mobility, while slower screw segments control loop growth. This disparity in mobility gives rise to asymmetric loops with long straight screw segments punctuated by edge kinks. As they grow, secondary loops intersect primary dislocations resulting in jogs and dislocation junctions. As the applied stress is increased further, some screw dislocation segments cross-slip onto complementary \{111\} planes. Interestingly, cross-slip is seen to occur according to the Fleischer mechanism [14] whereby a leading Shockley partial dislocation, say \( \frac{a}{2} \langle 211 \rangle \) (\( \gamma A \) in Thompson’s notation), dissociates into two partials according to the reaction

\[
\frac{a}{2} \langle 211 \rangle \rightarrow \frac{a}{4} \langle 110 \rangle + \frac{a}{4} \langle 110 \rangle
\]

Fig. 3. Cross-section through the center of the void showing the displacement field in the shear direction superposed on the adapted mesh at a shear angle of \( \theta = 6.9^\circ \) corresponding to the first yield point. Two oppositely-oriented discontinuities at \( 45^\circ \) to the principal void axes can be clearly observed, signaling the nucleation of partial dislocations.
One of these partials, $\beta A$, glides on the cross-slip plane whereas the remaining partial, $\gamma \beta$, is sessile. Further, the second of the Shockley partials, $D\gamma$, originally on the primary plane, is attracted to the sessile partial (stair-rod) and combines with it to give the second Shockley partial needed on the cross-slip plane, i.e.:

$$\frac{1}{6}[112] + \frac{1}{6}[10\bar{1}] \rightarrow \frac{1}{6}[211],$$

$$D\gamma + \gamma \beta \rightarrow \beta A.$$  \hspace{1cm} (3)

This reaction presumes cross-slip to occur onto the portion of the cross-slip plane making an acute angle with the primary plane, precisely as observed in simulations. Evidently, reactions (3) and (4) entail a certain activation energy that must be overcome by a corresponding increase in the applied stress. Cross-slip by a Fleischer mechanism runs counter to the accepted Friedel–Escaig cross-slip model for fcc metals [16], especially metals such as Al with relatively high stacking fault energy. In these metals, constriction is commonly thought to be favored due to the relatively short partial separation distance [21]. Additionally, some of the jogs developed at this stage grow, resulting in dislocation multiplication. Multiplication requires considerable mechanical work and, consequently, becomes important only at sufficiently high applied stress.

Stage III involves further nucleation and growth of secondary dislocation loops, as well as cross-slip of pre-existing dislocations. In order to keep up with the rapid loop growth, the atomistic-resolution region around the void must grow accordingly. Fig. 5 shows the shear component of the displacement field superposed on the adapted triangulation at the critical shear angle of $\theta = 11.3^\circ$, corresponding to an applied stress of $\tau_1 = 13.9$ GPa. The number of nodes in this mesh is 562,988 and the atomistic region extends over a radius of the order of 10 times the initial void radius. The displacement field exhibits a strong gradient in the vicinity of the void with two lobes at 45$^\circ$ angles to the principal cubic directions. The plane on which the displacement field is observed to invert its sign in the figure coincides with $\{111\}$ stacking faults in the crystal lattice, which in turn reveals the presence of partial dislocations. The high degree of distortion of the void is also noteworthy. Fig. 6 shows the corresponding dislocation structures. Large shear loops on the activated slip systems in addition to cross-slipped segments, jogs and dislocation junctions can be observed in this figure.

Following stage III, the dislocation activity around the void becomes exceedingly complex due to the juxtaposition and transformation of existing structures and the nucleation of new ones. Despite this complexity, screw-segment annihilation mediated by cross-slip is a clearly discernible mechanism in this state. At large applied strains, this process eventually results in dislocation density recovery and stress saturation (cf. Fig. 1).

It is interesting to note that the stages of deformation just described bear a qualitative resemblance with those observed in fcc single crystals oriented for single slip...
Thus, fcc single crystals exhibit a first stage of easy glide on primary slip systems, followed by a second stage of work hardening caused by the interaction between primary and secondary dislocations, and a final stage of recovery characterized by cross-slip and climb of screw dislocations. Likewise, the shear deformation of a nanovoid exhibits an initial phase of easy glide on primary slip planes, leading to the formation of strong obstacles and stress buildup. This phase is followed by secondary slip and work-hardening mechanisms such as jog, junction and lock formation.

3.2. Stress recovery phase

The unloading curve ($\tau_u, \theta$) is also shown in Fig. 1. As indicated by the closed cycles between the first and second yield points, $6.9^\circ < \theta < 9.1^\circ$, and between the second yield point and the last loaded configuration, $9.1^\circ < \theta < 11.3^\circ$, the plastic work within these intervals is expended in dislocation structures that are fully recovered. In particular, many of the shear loops generated on secondary slip planes during stage III and that, therefore, lie at distances relatively close to the void surface are entirely re-absorbed. This process is governed mainly by the distance of the secondary loops to the void surface, which in turn determines the magnitude of the image forces. The loop absorption occurs gradually, and is accompanied by volume recovery during the early stages of unloading (Fig. 9). By contrast, cross-slipped and jogged dislocation segments that have undergone irreversible transformations continue to evolve under the action of a positive applied stress, $\tau_u > 0$. Thus, screw dislocations of opposite sign continue to cross-slip and annihilate until the applied stress is reduced below a value too small to drive the process. These processes themselves result in a substantial dislocation density reduction, though this reduction does not translate into void volume recovery. As the shear stress approaches zero, image effects become the dominant driving force and even distant dislocations loops are gradually re-absorbed by the void surface. Complete unloading of the sample leaves a residual shear deformation of $\theta = 4.7^\circ$. When the stress finally reverses sign, the remaining dislocations are mechanically driven towards the void, assisted by image forces. However, structures that lie on planes that do not directly intersect the void surface survive and remain mostly unchanged during unloading. The residual dislocation structures are shown in Fig. 7, where heavily juggled short segments, as well as long dissociated segments revealing frequent cross-slip, can be observed. The corresponding residual displacement field is shown in Fig. 8. Isolated vacancies, represented in the figure as compact 12-atom clusters (the 12 nearest-neighbors whose centro-symmetry parameter is affected by the removal of an atom), are also present in Fig. 7, the direct result of stress-assisted jog-dragging episodes. There is some theoretical and experimental evidence that vacancies thus created may further enhance dislocation mobility in Al [23,24].
3.3. Void volume and shape evolution

The normalized void growth vs. shear angle ($\Delta V_v/V_{v0}$) curve is shown in Fig. 9. $\Delta V_v/V_{v0}$ denotes the relative void volume change with respect to the initial void volume of 72.9 nm$^3$. As discussed above, dislocation emission episodes result in marked stress drops in the macroscopic response curve. Notably, these bursts result in a net void volume decrease, i.e., mass transport occurs from the matrix towards the void, resulting from the vacancy character of all the dislocation structures observed. The total volume reduction of the void at the point of maximum shear is of the order of 9%, which is of the same order as the applied shear deformation. Since the applied macroscopic shear deformation is nominally volume-preserving, the change of volume of the void is strictly a finite-deformation effect. This is in contrast with the hydrostatic tension case, where void expansion is a first-order effect [8].

The analysis of the void shape sheds additional light on the deformation behavior of the void. An ideal void in a continuum starting with a spherical shape when $\gamma = \theta = 0$ evolves through a sequence of ellipsoidal shapes under the action of a remote shear deformation field. At the atomistic level, following the onset of plastic deformation the void surface develops discrete slip steps superimposed on the ideal ellipsoidal shape. Fig. 10 shows the evolution of the aspect ratio $b/a$ of the void as a function of shear angle. The aspect ratio $b/a$ is defined as the ratio between the lengths of the minor and major axes of the void. For simplicity, these are taken to coincide with the principal directions of deformation. The quotient $b/a$ measures the departure of the void shape from perfect sphericity and therefore initially has a value of one. We find that the aspect ratio decreases monotonically with $\theta$ during the loading stage, and exhibits a marked drop at the first recorded yield point at $\theta = 6.9^\circ$. The aspect ratio attains a minimum value of 0.66 at the maximum prescribed deformation. During the unloading stage the aspect ratio increases monotonically up to a final value of 0.96. This remnant nonsphericity occurs simultaneously with the incomplete void volume recovery shown in Fig. 9. The behavior just described is reminiscent of the analytical results of Fleck and Hutchinson [25] for a three-dimensional void in a viscoelastic solid subjected to simple shear, which predict an ostensibly linear variation of $b/a$ with $\theta$.

4. Summary and concluding remarks

We have analyzed the mechanisms underlying the deformation of a nanovoid in an Al crystal subjected to cyclic shear deformation. Boundary and cell-size effects have been minimized by means of the QC method. During the loading phase, our analysis reveals several stages of stress buildup separated by yield points. Stage I of deformation is elastic. The first yield point occurs at 4.3 GPa and corresponds to the formation of incipient dislocations on the surface of the void, at 45$^\circ$ to the principal void directions. The principal mechanisms underlying stage II of deformation are: glide of primary partial dislocation loops; and the reaction of the leading partial dislocations to form Lomer–Cottrell locks. An unexpected result of the simulations is that cross-slip occurs by the Fleischer mechanism and not by the more commonly assumed Friedel–Escaig mechanism. The second yield point corresponds to a burst in emission of dislocations on secondary planes. The principal mechanisms operating during stage III are: glide of secondary dislocations of mixed screw-edge character; dislocation intersection to form jogs and junctions; cross-slip; and dislocation multiplication and annihilation. During unloading, most of the dislocation population and void
volume reduction is recovered by re-absorption of dislocation loops and screw-segment annihilation. However, a residual dislocation density remains around the void at the end of the unloading process.

The limitations of the present analysis should also be carefully noted. Due to the emission of large numbers of dislocations, the atomistic region of the mesh grows steadily with deformation and, eventually, the size of the problem becomes unmanageably large. This limitation can be mitigated by recourse to mesh unrefinement, e.g., in the wake of moving dislocations. A particularly attractive additional possibility is to transition from quasicontinuum to dislocation dynamics far away from the void. Also, a more complete study of nanovoid deformation might consider the combined effects of mixed volumetric and shear deformation. Under those conditions, it is conceivable that the successive yield points identified in this study might extend to yield surfaces, e.g., in the pressure-shear plane. A complete charting of yield surfaces and deformation mechanisms for nanovoids deforming under combined pressure-shear would add greatly to current efforts in multiscale modeling of shock-induced spallation in metals.

Acknowledgment

Support from DOE through Caltech’s ASC/ASAP Center for the Simulation of the Dynamic Response of Materials is gratefully acknowledged.

References