Dynamic void collapse in crystals: computational modelling and experiments

By SIA NEMAT-NASSER, T1 MOO OKINAKA†, VITALI NESTERENKO and MINGQI LIU

Center of Excellence for Advanced Materials, Department of Applied Mechanics and Engineering Sciences, University of California at San Diego, La Jolla, CA 92093-0416, USA

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Abstract

Localization of inelastic flow and crack initiation in fcc single crystals are studied experimentally and by numerical simulations, focusing on the anisotropic inelastic response of the crystal, and the mechanism of possible crack initiation and growth, produced upon unloading by the residual inhomogeneous plastic strains. Hollow circular cylinders of single-crystal copper are subjected to externally applied explosive loads which cause the collapse of the cylinder; this procedure is called the thick-walled cylinder (TWC) method. Then, numerical simulations are performed to understand the deformation process which leads to localized deformation, and tensile cracking when partial collapse is followed by unloading. Various loads and initial orientations of the lattice are examined in these numerical simulations in order to study their effects on the flow localization and crack initiation phenomena.

§1. Introduction

The objective of this research is to study the localization of the inelastic flow and the possible subsequent crack propagation in single crystals experimentally and by numerical simulations, focusing on the anisotropic inelastic response and mechanisms of possible crack initiation and growth, produced upon unloading by the residual inhomogeneous plastic strains. A detailed study of such inelastic flow localization and crack propagation is important, since strain localization in single crystals can lead to global instability.

Localized deformation and shearbanding of ductile metals have been the subject of numerous investigations over the past few decades. Large plastic deformations often lead to failure by strain localization. The understanding of the behaviour of materials at large strains and high strain rates is of importance in metal forming, high-speed machining, high-velocity impact, crash-worthy design, penetration mechanics, explosive–metal interaction, and other similar dynamic phenomena.

In a recent paper, an experimental technique, called the ‘thick-walled cylinder (TWC) method’, has been used by Nesterenko et al. (1989,1991), to study strain localizations at high strain rates. The strain rate in the TWC method can be much higher than the strain rate which can be achieved by conventional methods, such as the Hopkinson bar technique. Nesterenko and Bondar (1994) observed

†Also at: Department of Civil Engineering, Kinki University, Japan.
shearbanding and cracking under high-strain and high strain-rate conditions in various polycrystalline materials, such as copper and niobium.

The dynamic void collapse and void growth in single crystals under uniform farfield stresses were studied analytically by Nemat-Nasser and Hori (1987), showing that tension cracks can be produced upon unloading in a direction normal to the applied compression. Nemat-Nasser and Chang (1990) followed this analytical work and experimentally illustrated the basic phenomenon using the Hopkinson bar technique. They observed that cracks propagate into the recrystallized grains at the nominal strain rate of about $10^4 \text{s}^{-1}$, which corresponds to local strain rates exceeding $10^6 \text{s}^{-1}$, near the boundaries of a collapsing void. Nemat-Nasser and Chang discuss the mechanism of the formation of Lomer–Cottrell sessile dislocations during loading, which can then lead to fracturing during unloading. Their scanning electron microscopy (SEM) seems to support this explanation. Cuínino and Ortiz (1996) seek to explore the possibility of vacancy condensation as a void-nucleating mechanism in fcc single crystals at large plastic deformations, and suggest that high strain rates inhibit void nucleation and promote brittle fracture in the experiments of Nemat-Nasser and Chang. An earlier analysis of Nemat-Nasser and Hori (1987) showed development of high tensile stresses at the tips of a collapsed void, once the applied compression is removed.

Here, we study the localization of inelastic flow and the subsequent crack propagation in fcc single crystals under uniform high strain-rate compressive loading. The TWC method is used in the experiment. A hollow cylindrical single-crystal copper specimen is subjected to high strain-rate uniform compressive loading. The loading condition is carefully chosen to ensure both the full and partial collapse of the specimen, inducing the flow localization and subsequent cracking of the specimen on unloading.

Then, numerical simulations are performed to explore the details of this process. A new algorithm to simulate finite deformation of fcc single crystals, proposed by Nemat-Nasser and Okinaka (1996), is implemented into the finite-deformation code, DYNA2D, and used for the simulation. Various loads and initial configurations of the lattice are examined in these numerical simulations in order to study their effects on the flow localization and subsequent crack initiation phenomena.

§2. Experimental procedure and results

Externally applied explosives are used to collapse a thick-walled cylinder of single-crystal copper. The specimen consists of a hollow cylindrical tube of single-crystal copper encased in a polycrystal copper jacket. The single-crystal tube is cut from a single-crystal rod, using a spark erosion technique. Then, the sample is loaded by detonating an explosive which surrounds the specimen cell. The magnitude of the explosive is carefully chosen to ensure either full or partial collapse of the hollow cylindrical specimen. The size and shape of the hollow cylindrical specimen, and the overall experimental set-up for the TWC method are shown in figures 1 and 2, respectively. The initial configuration of the single crystal is measured from the remaining part of the sample, using X-ray diffraction. The axis of the cylinder is found to be in the $[1\overline{3}4]$ direction.

In the first experiment, the hollow cylindrical single-crystal specimen is fully collapsed under conditions which have been discussed by Nesterenko and Bondar (1994). The detonation speed measured in this particular experiment was $D = 4030 \text{ms}^{-1}$ (explosive ammonite + sand (10%vol.) with density $1 \text{gcm}^{-1}$),
Figure 1. Shape and size of the specimen used in the experiment.

Figure 2. Experimental setup.
with the diameter of the explosive charge being 60 mm. The estimated detonation pressure

\[ P = \frac{\rho T^2}{\kappa + 1}, \quad \kappa \approx 3 \]  

is about 4 GPa. The initial radial velocity of the inner boundary of the specimen is measured by the non-contact electromagnetic method and is about 200 ms\(^{-1}\), leading to a time of collapse of about 8 ms.

Optical micrographs of the overall and the central region of the collapsed specimen are shown in figures 3 and 4, respectively. Figure 3 shows that the outer

![Figure 3. Optical micrograph of the fully collapsed specimen.](image)

![Figure 4. Optical micrograph of the central part of the fully collapsed specimen. The central crack is the inner boundary of the collapsed cylinder. The lines around the central curve indicate flow localization zones.](image)
boundary of the collapsed specimen is non-circular. The lines of the shearbanding, running from the outer boundary to the collapsed inner boundary, are also seen in this figure. In figure 4, the central curved lines are the inner boundary of the cylinder. Lines of the flow localization are also observed around the central crack in this picture. Since the shape of the outer part of the jacket of the specimen and the loading condition are axially symmetric, it can be concluded that the localization is caused by the anisotropic inelastic response of the single crystal.

Next, the loading condition is estimated for a partially collapsed specimen, and is used to simulate the crack initiation and propagation which occur upon unloading. To ensure an incomplete void collapse, a suitably smaller explosive loading was chosen. The outer diameter of the explosive charge was decreased to 55mm, resulting in a smaller detonation speed of about $D = 3030 \text{ms}^{-1}$. According to (1), this gives a detonation pressure of about 2.3 GPa, leading to an incomplete collapse.

The overall configuration of the deformed specimen is shown in figure 5, with the central part of the specimen magnified in figure 6 for detailed observation. These pictures are, again, taken using an optical microscope. The outer boundary develops a non-circular shape after unloading. The inner boundary, which has a circular shape initially, develops a rectangular shape, and cracks are initiated at four corners of the rectangle. Shearbands develop around the four cracks, and also, from the outer boundary to the upper and bottom segments of the inner boundary of the cylinder. However, the mechanism of crack initiation and propagation is not revealed by these observations. Hence, numerical simulations are used to examine this process and to develop a detailed understanding of the phenomenon.

![Optical micrograph of the partially collapsed specimen.](image-url)
§3. Numerical simulations

3.1. Kinematics and constitutive relations

In this subsection, first, the fundamentals of the general kinematics, on which the numerical calculation is based, are briefly reviewed. The general kinematics of the elastic–plastic deformation of crystals at finite strains is given by Hill (1966), Rice (1970), Hill and Rice (1972), and others. Reviews are given by Nemat-Nasser (1983), Asaro (1983), and Havner (1992).

The total deformation gradient, \( \mathbf{F} \), is divided into a non-plastic (elastic plus rigid-body rotation) deformation gradient, \( \mathbf{F}^* \), and a plastic deformation gradient, \( \mathbf{F}^p \), as follows:

\[
\mathbf{F} = \mathbf{F}^* \mathbf{F}^p.
\]  

(2)

The velocity gradient is defined by

\[
\mathbf{L} = \dot{\mathbf{F}} \mathbf{F}^{-1},
\]

(3a)

where the dot stands for the time derivative. Similarly, the non-plastic velocity gradient, \( \mathbf{L}^* \), and the plastic velocity gradient, \( \dot{\mathbf{L}}^p \), are given by

\[
\mathbf{L}^* = \dot{\mathbf{F}}^* \mathbf{F}^{*{-1}},
\]

(3b)

and

\[
\dot{\mathbf{L}}^p = \mathbf{F}^p \mathbf{F}^{p^{-1}},
\]

(3c)
where the hat is used to denote that the velocity gradient is measured with respect to the initial configuration of the crystal lattice. Substitution of (2), (3 b), and (3 c) into (3 a) yields

$$L = L^* + F^* \dot{L}^P F^{*-1}. \quad (3 \text{d})$$

It is assumed in this work that the plastic deformation is solely due to the crystalline slip. Hence, the plastic velocity gradient, \( \dot{L}^P \), is given by the sum of the slips of all slip systems. Since fcc single crystals have four slip planes and three slip directions on each plane, it follows that

$$\dot{L}^P = \sum_{\alpha=1}^{4} \sum_{a=1}^{3} \gamma^{(\alpha \nu)} l_0^{(\alpha \nu)}, \quad (4)$$

where \( \gamma^{(\alpha \nu)} \) is a slip rate, and \( l_0^{(\alpha \nu)} \) is the \( a \)th slip direction on the \( \alpha \)th slip plane, which is defined by

$$l_0^{(\alpha \nu)} = s_0^{(\alpha \nu)} \otimes n_0^{(\alpha \nu)}. \quad (5)$$

Here, \( s^{(\alpha \nu)} \) and \( n^{(\alpha \nu)} \) are the slip direction and the slip plane normal, respectively, and the subscript 0 stands for the initial configuration of the lattice.

Since the elastic strains are generally small, it is reasonable to neglect them in comparison with the lattice rotation. Hence, from (3 d) and (4), obtain

$$L = L^* + \sum_{\alpha=1}^{4} \sum_{a=1}^{3} \gamma^{(\alpha \nu)} l^{(\alpha \nu)}, \quad (6 \text{a})$$

where

$$l^{(\alpha \nu)} = R^* l_0^{(\alpha \nu)} R^{*T}, \quad (7)$$

and \( R^* \) is the lattice rotation tensor. With small elastic strains, the non-plastic velocity gradient becomes

$$L^* = \dot{\varepsilon} + \varepsilon \Omega^* - \Omega^* \dot{\varepsilon} + \Omega^*, \quad (8)$$

where \( \varepsilon \) is the lattice elastic strain, measured in the rotated lattice, and \( \Omega^* \) is the lattice spin rate defined by

$$\Omega^* = \dot{R}^* R^{*T}. \quad (9)$$

The symmetric and antisymmetric parts of (6 a) are given by

$$D = D^* + \sum_{\alpha=1}^{4} \sum_{a=1}^{3} \gamma^{(\alpha \nu)} p^{(\alpha \nu)}, \quad (6 \text{b})$$

and

$$W = W^* + \sum_{\alpha=1}^{4} \sum_{a=1}^{3} \gamma^{(\alpha \nu)} w^{(\alpha \nu)}, \quad (6 \text{c})$$

where \( D^* \) and \( W^* \) are the symmetric and antisymmetric parts of the non-plastic velocity gradient, \( L^* \), respectively. Also, \( p^{(\alpha \nu)} \) and \( w^{(\alpha \nu)} \) are the symmetric and antisymmetric parts of the slip system tensor, \( l^{(\alpha \nu)} \), respectively.

Linear elasticity is used to model the elastic lattice distortion,

$$\sigma = C^* : D^*, \quad (10)$$
where $\sigma$ and $C^*$ are the Jaumann rate of the Cauchy stress and the elasticity tensor in the rotated lattice, respectively.

The rate-dependent slip model with the power law is employed to model the crystalline slip. Hence, the slip rate of the $(\alpha \ell)$th slip system is assumed to be given by

$$\dot{\gamma}^{(\alpha \ell)} = \dot{\gamma}_0^{(\alpha \ell)} \left| \frac{\tau^{(\alpha \ell)}}{\tau_Y^{(\alpha \ell)}} \right|^m,$$

(11)

where $\tau^{(\alpha \ell)} = \langle \sigma, p^{(\alpha \ell)} \rangle$ is the resolved shear stress, and

$$\text{sgn}(x) = \begin{cases} 1 & \text{for } x \geq 0, \\ -1 & \text{for } x < 0. \end{cases}$$

(12)

In equation (11), $\tau_Y^{(\alpha \ell)}$ and $\dot{\gamma}_0^{(\alpha \ell)}$ are the critical resolved shear stress and the reference value of the slip rate, respectively. A linear strain-hardening model is considered. The critical resolved shear stress, $\tau_Y^{(\alpha \ell)}$, is thus expressed as

$$\tau_Y^{(\alpha \ell)} = \sum_{\beta=\alpha}^{4} \sum_{\beta_b=1}^{3} h(\gamma)^{(\alpha \ell)}_{(\beta \beta_b)} \dot{\gamma}^{(\beta \beta_b)},$$

(13a)

where

$$\dot{\gamma} = \sum_{\alpha=1}^{4} \int \left| \gamma^{(\alpha \ell)} \right| d\xi$$

(13b)

While thermal softening can be included in the power-law model, as in Nemat-Nasser et al. (1993), this effect is neglected in the present case, since the flow stress of copper is relatively small and its heat conductivity is rather high.

An efficient algorithm to solve (6b) incrementally for a given constant $D$ has been proposed by Nemat-Nasser and Okinaka (1996). They exploit the physical fact that large deformations of metals are due to plastic flow with only a very small accompanying elastic contribution when five linearly independent slip systems are active. Based on this, an efficient algorithm is proposed by these authors by combining the plastic-predictor elastic-corrector method and a conventional implicit or explicit time-integration scheme. In the present work, this new algorithm is implemented into the finite-deformation code DYNA2D, and is used to simulate the cylinder-collapse experiments numerically.

§4. NUMERICAL SIMULATION OF THE FULLY COLLAPSED CYLINDER

The initial mesh of the hollow cylindrical specimen is shown in figure 7. Only the single-crystal specimen is simulated. The polycrystalline jacket is not included in this analysis, but its effect is represented as boundary conditions on the single crystal. The mesh includes 5760 elements with 5904 nodes. Although each element has the same crystal orientation initially, it develops its own crystal orientation during the deformation, and hence, a very fine mesh is required. The initial configuration of the lattice in this simulation is chosen to correspond to the experiment, i.e. the $[13 4]$ plane. The $x$ and $y$ axes are arbitrarily chosen to coincide with the $[25 3 4]$ and $[0 4 3]$ directions in terms of the Miller indices. In the numerical simulation, the inner boundary is defined as a contact surface without friction.
The loading condition is defined in terms of the velocity of the nodes on the outer boundary of the single-crystal cylinder. Hence, nodes on the outer boundary move toward the centre of the specimen with the prescribed velocity, maintaining a circular shape for this boundary. The velocity of these nodes is obtained as follows: first, it is assumed that the hollow cylindrical specimen fully collapses at $t_c = 8.5\, \mu s$ with zero volumetric strain under plane strain conditions. The total travelling distance of the outer boundary is, then, given by

$$
\int_0^{t_c} v_r(t) \, dt = 2.02 \times 10^{-3} \, \text{m},
$$

where

$$
v_r = \frac{dr_t}{dt}.
$$

The initial velocity is given by

$$
v_r(0) = 150 \, \text{m} \, \text{s}^{-1}.
$$

The time-variation of the radial velocity, $v_r(t)$, is approximated by

$$
v_r(t) = A_0 \exp\left[-\alpha(t - t_0)^2\right].
$$

Then, if we require that (14) and (16) are satisfied at $t_0 = 4.0\, \mu s$, it follows that $\alpha = 0.044$ and $A_0 = 0.303274$. Hence, we obtain

$$
v_r(t) = 0.303274 \exp\left[-0.044(t - t_0)^2\right].
$$

This curve is plotted in figure 8. In the simulation, the points marked in this figure are given, and they are linearly interpolated to define the loading curve.
Next, the material property used in the simulation is discussed. Although the single-crystal copper is *elastically* anisotropic, its effect for large plastic strains and rotations is insignificant relative to that of the inelastic anisotropy, and hence, elastically isotropic material is assumed. The shear modulus and Poisson’s ratio are \( \mu = 45 \text{GPa} \), and \( \nu = 0.33 \), respectively. The rate-sensitivity power in (8) is set at \( m = 101 \). The initial value of the critical resolved shear stress is assumed to be 0.25% of the elastic shear modulus, so that \( \tau_{Y_0} = 112.5 \text{MPa} \). For the strain hardening, the rate of change of the critical resolved shear stress is

\[
\dot{\tau}^{(\alpha)} = \frac{4}{\beta} \sum_{\beta=1}^{3} h_{(\beta \beta)}^{(\alpha \alpha)} \left| \gamma^{(\beta \beta)} \right|.
\]  

(19)

Here,

\[
h_{(\beta \beta)}^{(\alpha \alpha)} = h(\gamma) \left( \delta_{(\beta \beta)}^{(\alpha \alpha)} + r(1 - \delta_{(\beta \beta)}^{(\alpha \alpha)}) \right),
\]

(20)

where

\[
h(\gamma) = \begin{cases} 
0.003125 \mu & \gamma \leq 0.32, \\
\frac{0.003125 \mu}{1.0 + 3.7 (\gamma - 0.32)} & \gamma > 0.32,
\end{cases}
\]

(21)

\[
\gamma = \sum_{\alpha=1}^{4} \sum_{a=1}^{3} \left| \tau^{(\alpha \alpha)} \right| d\xi
\]

(22)

Figure 8. Loading condition used in the simulation.
and \( r = 1.25 \) is used. This assumes that the latent hardening exceeds self-hardening by 25\%. With this strain hardening, the critical resolved shear stress levels off at three times its initial value, after a 200\% equivalent strain.

In the first simulation, the cylinder is fully collapsed at 8.1 ms. The overview and the magnified central part of the deformed mesh are shown in figure 9. In figure 9(a), the outer boundary of the collapsed specimen has a circular shape. As will be shown for the partially collapsed case, this is due to the plastic flow which continues after a complete collapse. The central part of the collapsed mesh in figure 9(b) is shown for comparison with the results of the experiment, figure 4. These two figures show good agreement, and hence it is concluded that the central curve in the experiment is the collapsed inner boundary of the cylinder and not cracks originating from the centre.

Figure 9. Final deformation state of the fully collapsed specimen at 8.1 ms: (a) overall configuration, and (b) central part.
The lines of the flow localization are also observed around the central part of the collapsed cylinder.

In order to study the process of flow localization, the deformation states at 6.75 µs, 7.25 µs, and 7.75 µs are plotted in figures 10(a)–(c), respectively. The flow localization initiates at about 6.74 µs, when the initially circular inner boundary develops localization at four corners. The inner boundary then develops two parallel
straight and two semicircular edges. It is observed that, among the four segments, two shrink much faster after initiation of the localization. Although the loading on the outer boundary is uniform, the anisotropic inelastic response of the single crystal leads to a non-uniform shrinking speed of the inner boundary, and hence localization at the junction of the resulting segments.

The maximum and minimum principal stresses at 8.1 $\mu$s are shown in figures 11(a) and 11(b), respectively. In these figures, the unit of stress is MPa, and tension is positive. It is not possible to obtain the details of the stress distribution from the present simulation, since various important factors, such as thermal softening and frictional contact at the inner boundary, are not included in the simulation. However, it is clearly observed that large tensile stresses develop within the localized regions. These stresses are sufficient to cause crack initiation at the inner surface of the collapsed cylinder.

![Figure 11](image)

Figure 11. Contours of the (a) maximum and (b) minimum principal stresses.
Although the inelastic flow localization around the inner boundary is well simulated, the non-circular shape of the outer boundary, which is shown in figure 3, is not explored numerically, as the uniform loading is continued until the cylinder is fully collapsed. In another simulation, the loading on the outer boundary is removed at 5.5 ms, rendering the outer boundary traction free. Then, the cylinder is seen to fully collapse at 8.328 ms. The overall configuration and central part of the deformed mesh are shown in figure 12. The inelastic flow localization around the central part of the collapsed cylinder, which is shown in figure 12(b), is not significantly different from the last simulation (figure 9), while the shape of the outer boundary (figure 12(a)) shows a significant difference. The experimentally observed non-circular shape of the outer boundary (figure 3) is well simulated. Here, it is noted that the given loading condition is uniform on the outer boundary until the loading is removed, and hence, this non-circular shape observed here is solely due to the anisotropic inelastic response of the single crystal.

Figure 12. Final deformation state of 8.328 ms: (a) overall configuration and (b) central part.
In order to study the effect of the initial configuration of the lattice on the flow localization, two other initial lattice configurations are examined. As the first configuration, a (0 0 1) cylinder is considered. The cross-sectional area is the (0 0 1) plane, and the \( x \) and \( y \) axes coincide with the [1 0 0], and [0 1 0] directions, respectively. Due to the crystal symmetry of fcc single crystals, the \( x \), \( y \) axes and the lines \( y = \pm x \), are the axes of symmetry in this cylinder. As the second configuration, a (1 1 1) cylinder is examined. The cross-sectional area is the (1 1 1) plane, and the \( x \) and \( y \) axes coincide with the [1 1 0], and [1 1 2] directions, respectively. The (1 1 1) plane in the fcc single crystal is the plane with the highest symmetry. The (1 1 1) cylinder has six axes of symmetry, the \( x \), \( y \) axes and the lines \( y = \pm 3^{-1/2} x \) and \( y = \pm 3^{1/2} x \). In both simulations, the mesh size is the same as the one used for the (1 3 4) cylinder, and the loading is continued according to the velocity curve shown in figure 8, until the cylinder is fully collapsed. However, only the first quadrant is considered, because of the symmetry of the deformation.

![Figure 13. Final deformation state of the (001) cylinder at 8.15 μs: (a) overall configuration and (b) central part.](image)

(a) Overall Configuration

(b) Central Part
The overall configuration and the central part of the deformed meshes at 8.15 ms are shown in figures 13 and 14, for the (001) and (111) cylinders, respectively. Figures 13(b) and 14(b) are shown for comparison with figure 9(b). While in these simulations, fourfold and sixfold symmetries are expected, due to inaccuracy in the calculations of the contact surface, this symmetry is not maintained in figures 13 and 14. Localization of the inelastic flow in these simulations is a result of the anisotropic inelastic response of the single crystal. Since the anisotropy has a significant dependency upon the initial configuration of the lattice, the difference in the initial configurations creates such remarkable differences in the flow localization.

In order to study the initiation of the flow localization, the deformation states at 6.75 ms, 7.25 ms, and 7.75 ms are plotted in each simulation; see figure 15 for the (001) cylinder and figure 16 for the (111) cylinder. Unlike the (134) cylinder, the inner boundaries of the (001) cylinder and the (111) cylinder develop into an octahedral and a hexagonal shape, respectively. These shapes satisfy the required
symmetry associated with the initial lattice orientation, since at these stages of deformation there are no contact surfaces. These shapes are not unique, and some other shapes can also satisfy the required symmetry. Hence, materials other than copper which have different properties may develop different shapes upon collapse, starting from a common initial configuration.

§5. Numerical simulation of the partially collapsed cylinder

Partially-collapsed cylinders (figures 5 and 6) offer unique features whose study requires special consideration. Crack initiation on unloading in single crystals under uniform compression, is one such feature which is examined in this subsection. The initial mesh for this simulation is shown in figure 17. It includes 2800 elements with 2940 nodes. The initial configuration of the lattice coincides with the experimental sample, the cross-sectional area being the (1 3 4) plane. Again, the $x$ and $y$ axes are arbitrarily chosen, so that they coincide with the [25 3 4], and [0 4 3] directions, respectively. Nodes on the outer boundary are moved toward the centre of the specimen with the given velocity, as shown in figure 8, until 1.1 $\mu$s. The given loading

Figure 15. Deformation state of the (001) cylinder at (a) 6.75 $\mu$s, (b) 7.25 $\mu$s and (c) 7.75 $\mu$s.
Figure 16. Deformation state of the (111) cylinder at (a) 6.75 µs, (b) 7.25 µs and (c) 7.75 µs.

Figure 17. Initial mesh used in the numerical simulation.
condition is then removed, rendering the outer boundary traction-free. This leads to an incomplete collapse of the cylinder.

The overall configuration and the central part of the deformed mesh at 40 μs, are shown in figure 18. Figure 18(b) shows excellent correlation with the results of the experiment, shown in figure 6. It is noteworthy that the similarity between the simulation and the experiment is observed not only in the flow localization around the inner boundary, but also in the shape of the outer boundary after unloading. The non-circular shape of the outer boundary of the unloaded specimen, shown in figure 5, has been one of our main concerns, since it might have been caused by the variation of the explosive loading, although a uniform loading may be expected. However, comparison with simulation reveals that this geometry is caused by the anisotropic inelastic response of the single crystal.

![Figure 18](image)

(a) Overall Configuration

(b) Central Part

Figure 18. Final deformation state of the (1 3 4) cylinder at 40.0 μs: (a) overall configuration and (b) central part. Loading is removed at 1.1 μs in this simulation.
Figure 19. Deformation state of the (001) cylinder at (a) 10.0 μs, (b) 12.5 μs and (c) 15.0 μs.

Figure 20. Expansion of the inner boundary: bold and fine lines are the inner boundaries at 18.0 μs and 20.0 μs, respectively.
In order to study the initiation of the flow localization, the deformation states at 10.0 μs, 12.5 μs, and 15.0 μs are plotted in figure 19 for the (001) cylinder. Although the loading is removed at 1.1 μs, the hollow cylindrical specimen keeps shrinking until about 20.0 μs. The flow localization is initiated at about 10.0 μs, as shown in figure 19(a). Then, flow localization develops at four corners on the inner boundary, as shown in figures 19(b) and 19(c).

At the end of this section, crack propagation is discussed. The hollow cylinder experiences a maximum compaction at around 18.0 μs, and then starts to expand. The expansion of the inner boundary is shown in figure 20. In this figure, the thick and thin lines are the inner boundaries at 18.0 μs and 20.0 μs, respectively. Although the total expansion is small when compared with the total deformation, it opens the folds of the inner boundary, and hence, produces large tensile stresses around the sharp tips of the folded inner boundaries.

Next, the tensile stresses caused by the expansion are considered by examining the maximum principal stresses in elements around the flow localization regions. Since the total deformation is almost centrally symmetric, only two parts, denoted by A and B, are considered. The positions of the considered parts within the overall mesh are shown in figure 21(a). These two parts are magnified and the element numbers in each part are shown in figures 21(b) and 21(c), respectively.

![Overall configuration of the deformed mesh, and elements around the fold.](image)

(a) Overall configuration: Two parts, A and B are shown.

(b) Elements in Part A.

(c) Elements in Part B.

Figure 21. Overall configuration of the deformed mesh, and elements around the fold.
Figure 22. Maximum principal stresses in part A. Stresses in the elements around (a) the larger fold and (b) the smaller fold.
The inner boundary in part A has two folds, and hence, the maximum principal stresses in elements around these two folds are calculated and plotted. The maximum principal stresses in five elements around the larger fold are shown in figure 22(a), and those in three elements around the smaller fold are shown in figure 22(b). In figure 22(a), the maximum tension seems to occur in element 714 at 18.165 µs, and its magnitude is 2.7 GPa. Such a remarkable tensile stress does not occur in figure 22(b). Similarly, the maximum principal stresses in part B are plotted in figure 23. The maximum tension of 3.39 GPa occurs in element 22 at 25.31 µs. Although dynamic crack propagation under the high-strain, high strain-rate conditions has not been well studied, it may be reasonable to conclude that such large tensile stresses, caused by the expansion of the specimen upon unloading, initiate and propagate cracks which are observed in the experiment. Similar crack propagations have been observed by Nemat-Nasser and Chang (1990) in single-crystal copper, where a cylindrical hole has been collapsed in uniaxial compression at high strain rates. Tensile cracks have been observed to occur normal to the applied compression pulse. These authors conclude that these cracks are developed at the locked dislocations upon unloading.

§6. Conclusion

Localization of inelastic flow in fcc single crystals is studied experimentally and by numerical simulations. The TWC (thick-walled cylinder) method is used in the experiment. Numerical simulations are performed to examine the deformation process which leads to the observed final configuration. The new algorithm, proposed by Nemat-Nasser and Okinaka (1996), is implemented into the finite-deformation code, DYNA2D, in order to perform these simulations. Various initial configurations of the lattice are examined in the numerical simulation to study their effect on the flow localization phenomena.
The flow localization in fcc single crystals due to their anisotropy inelastic response is observed experimentally. The process of the localization is studied in detail through numerical simulations, and the comparison of the results with those of experiments shows remarkable agreements. It is also shown that the initial configuration of the lattice has a considerable effect on the flow localization phenomena.

Crack initiation and propagation in fcc single crystals are observed in experiments, and successfully simulated by numerical calculations. Through the numerical simulation, it is concluded that cracks are produced during the unloading process by the tensile stresses which are produced by large heterogeneous plastic deformations that occur during the loading regime.

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REFERENCES