

ANALYSIS OF DYNAMIC SHEAR BANDS IN AN FCC SINGLE CRYSTAL

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Abstract—We study plane strain dynamic thermomechanical deformations of an fcc single crystal compressed along the crystallographic direction $[010]$ at an average strain rate of 1000 sec^{-1} . Two cases are studied; one in which the plane of deformation is parallel to the plane (001) of the single crystal, and another one with deformation occurring in the plane $(10\bar{1})$ of the single crystal. In each case, the 12 slip systems are aligned symmetrically about the two centroidal axes. We assume that the elastic and plastic deformations of the crystal are symmetrical about these two axes. The crystal material is presumed to exhibit strain hardening, strain-rate hardening, and thermal softening. A simple combined isotropic–kinematic hardening expression for the critical resolved shear stress, proposed by Weng, is modified to account for the affine thermal softening of the material. When the deformation is in the plane (001) of the single crystal, four slip systems $(111)[1\bar{1}0]$, $(1\bar{1}\bar{1})[1\bar{1}0]$, $(1\bar{1}\bar{1})[110]$, and $(1\bar{1}1)[110]$ are active in the sense that significant plastic deformations occur along these slip systems. However, when the plane of deformation is parallel to the plane $(10\bar{1})$ of the single crystal, slip systems $(1\bar{1}1)[110]$, $(1\bar{1}1)[011]$, $(111)[1\bar{1}0]$, and $(111)[0\bar{1}1]$ are more active than the other eight slip systems. At an average strain of 0.108, the maximum angle of rotation of a slip system within a shear band, about an axis perpendicular to the plane of deformation, is found to be 20.3° in the former case, and 22.9° in the latter.

I. INTRODUCTION

One way to understand the micromechanics of shear band formation in polycrystalline materials is to study their initiation and growth in a single crystal. Several investigators, e.g. SAWKILL and HONEYCOMBE [1954], PRICE and KELLY [1964], SAIMOTO *et al.* [1965], and CHANG and ASARO [1981], have observed regions of localized shearing in fcc single crystals deformed quasistatically. ZIKRY and NEMAT-NASSER [1990] have recently studied numerically the phenomenon of shear banding in an fcc single crystal undergoing plane-strain tensile deformations at high strain rates. We refer the reader to their article for a list of references and a brief outline of the historical development of the subject. They used the double cross-slip model proposed by KOEHLER [1952] and later by OROWAN [1954] during the entire loading history. Here we study a similar problem with the crystal deformed in compression rather than tension, assume that all 12 slip systems are potentially active at any instant of loading, use constitutive relation for the critical shear stress that is different from the one employed by ZIKRY and NEMAT-NASSER [1990], employ a different technique to integrate the system of equations, and consider two loadings. With the axis of compression aligned along the crystallographic direction $[010]$, the plane of deformation is taken to be either parallel to the plane (001) or $(10\bar{1})$ of the single crystal.

When the plane of deformation is parallel to the plane (001) of the single crystal, a single shear band making an angle of 45° with the horizontal line ensues from the centroid of the cross-section and is reflected back from the top loading surface, the angle of reflection being essentially equal to the angle of incidence. The slip strains on the slip systems $(111)[1\bar{1}0]$, $(1\bar{1}\bar{1})[1\bar{1}0]$, $(1\bar{1}\bar{1})[110]$, and $(1\bar{1}1)[110]$ are high, and these constitute

the primary slip systems. At a nominal strain of 0.108, the maximum angle of rotation of the crystal lattice in the central and reflected bands equal 18.54° counterclockwise and 20.29° clockwise, respectively. When the plane of deformation is parallel to the plane $(10\bar{1})$ of the single crystal, the shear band originating from the center of the cross-section makes an angle of 39.5° with the horizontal, and eventually splits into two bands. Slip systems $(111)[1\bar{1}0]$ and $(111)[0\bar{1}1]$ in both the central and the reflected bands, and slip systems $(1\bar{1}1)[110]$ and $(1\bar{1}1)[011]$ in the reflected band are found to be more active than other slip systems.

II. FORMULATION OF THE PROBLEM

We use a set of fixed rectangular Cartesian coordinates to describe the thermomechanical deformations of an fcc single crystal of square cross-section and compressed along the crystallographic direction $[010]$ which is taken to coincide with the x_3 -axis. We assume that the x_1 - x_2 plane of deformation is either parallel to the plane (001) or $(10\bar{1})$ of the single crystal. In each case, the 12 slip systems are aligned symmetrically about the two centroidal axes. We presume that both elastic and plastic deformations of the single crystal are symmetric about the two centroidal axes, even after the band has formed, and accordingly study deformations of the material in the first quadrant only. In Eulerian description, equations governing the deformations of the single crystal are:

The balance of mass:

$$\dot{\rho} + \rho v_{i,i} = 0, \quad (1)$$

The balance of linear momentum:

$$\rho \dot{v}_i = \sigma_{ij,j}, \quad (2)$$

The balance of internal energy:

$$\rho c \dot{\theta} = -q_{i,i} + \sigma_{ij} D_{ij}^p, \quad (3)$$

where ρ is the present mass density, v_i the velocity of a material particle, a comma followed by i indicates partial differentiation with respect to the present position x_i of a material particle, σ_{ij} is the Cauchy stress tensor, a superimposed dot indicates the material time derivative, a repeated index implies summation over the range of the index, c is the constant specific heat, θ the temperature rise, q_i the heat flux per unit deformed area, and D_{ij}^p is the plastic part of the strain-rate tensor D_{ij} , defined as

$$D_{ij} = \frac{1}{2} (v_{i,j} + v_{j,i}). \quad (4)$$

D_{ij}^p is determined by the local plastic slip rate of all active slip systems at a material particle, and will be defined later. For plane strain deformations in the x_1 - x_2 plane, various quantities are functions of x_1 , x_2 and time t , and subscripts i, j range over 1 and 2. However, in the second term on the right-hand side of eqn (3), indices i and j extend to 3, since in plane strain deformations $\sigma_{33} \neq 0$ in general, and D_{33}^p need not equal zero during the plastic deformation. In eqn (3) we have assumed that all of the plastic working is converted into heating.

We now describe the constitutive relations for high strain-rate finite deformations of rate-dependent single crystals. We postulate Fourier's law of heat conduction, *viz.*

$$q_i = -k\theta_{,i}, \quad (5)$$

where k is the thermal conductivity, and is assumed to be independent of the deformation and temperature of the single crystal. We assume that the strain-rate tensor D_{ij} and the spin tensor W_{ij} defined as

$$W_{ij} = \frac{1}{2}(v_{i,j} - v_{j,i}) \quad (6)$$

have additive decompositions into elastic and plastic parts, *viz.*

$$D_{ij} = D_{ij}^e + D_{ij}^p, \quad W_{ij} = W_{ij}^e + W_{ij}^p. \quad (7)$$

The Cauchy stress rate corotational with the elastic distortion of the single crystal is assumed to be related to the elastic distortion rate by Hooke's law. That is,

$$\dot{\sigma}_{ij}^e = L_{ijkl} D_{kl}^e, \quad (8)$$

where

$$\dot{\sigma}_{ij}^e = \dot{\sigma}_{ij} + \sigma_{ik} W_{kj}^e - W_{ik}^e \sigma_{kj}, \quad (9)$$

and L_{ijkl} is the fourth order tensor of the elasticities of the single crystal. Here we take the crystal lattice to be elastically isotropic. Thus,

$$L_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}),$$

where λ and μ are Lamé's constants for the crystal material. Recall that the Jaumann stress rate $\dot{\sigma}_{ij}$ given by

$$\dot{\sigma}_{ij} = \dot{\sigma}_{ij} + \sigma_{ik} W_{kj} - W_{ik} \sigma_{kj}, \quad (10)$$

is corotational with the material element. Equations (7), (8), (9), and (10) result in

$$\dot{\sigma}_{ij} = L_{ijkl}(D_{kl} - D_{kl}^p) + \sigma_{ik} W_{kj}^p - W_{ik}^p \sigma_{kj}. \quad (11)$$

The Schmid stress or the resolved shear stress $\tau^{(\alpha)}$ of the α th slip system is assumed to be related to the local Cauchy stress σ_{ij} through

$$\tau^{(\alpha)} = \nu_{ij}^{(\alpha)} \sigma_{ij}, \quad (12)$$

where the Schmid factor $\nu_{ij}^{(\alpha)}$ is defined as

$$\nu_{ij}^{(\alpha)} = \frac{1}{2} (b_i^{(\alpha)} n_j^{(\alpha)} + b_j^{(\alpha)} n_i^{(\alpha)}), \quad (13)$$

$b^{(\alpha)}$ and $n^{(\alpha)}$ being the unit slip direction and the unit normal to the slip-plane of the α th slip system.

For a strain rate-dependent material of the single crystal, the slip rate of the α th slip system is assumed to be related to the resolved shear stress by the power law.

$$\dot{\gamma}^{(\alpha)p} = \begin{cases} \dot{\gamma}_0^{(\alpha)} \left[\frac{\tau^{(\alpha)}}{\tau_c^{(\alpha)}} \right] \left[\frac{|\tau^{(\alpha)}|}{\tau_c^{(\alpha)}} \right]^{1/m-1}, & \tau^{(\alpha)} \geq \tau_c^{(\alpha)}, \\ 0, & \tau^{(\alpha)} < \tau_c^{(\alpha)}, \end{cases} \quad (14a)$$

$$(14b)$$

where m is the rate sensitivity parameter, and $\dot{\gamma}_0^{(\alpha)}$ is a reference shear strain rate such that if the crystal is to be deformed with each $\dot{\gamma}^{(\alpha)p}$ set equal to $\dot{\gamma}_0^{(\alpha)}$, then $\tau = \tau_c^{(\alpha)}$ (PAN & RICE [1983]). When the resolved shear stress of the α th slip system is below the critical resolved shear stress $\tau_c^{(\alpha)}$ required to cause plastic deformation on that slip system, the α th slip system is taken to be inactive. The critical resolved shear stress is assumed to be a function of the initial flow stress τ_0 , work hardening, and the temperature θ . A simple combined isotropic-kinematic hardening expression for τ_c , proposed by WENG [1980], is modified as follows

$$\tau_c^{(\alpha)} = \left\{ \tau_0 + \sum_{\beta} [g + (1 - g) \cos \psi \cos \phi] h^{(\alpha\beta)} (\dot{\gamma}^{(\beta)p})^n \right\} (1 - \nu \theta) \quad (15)$$

to include thermal softening. In eqn (15), ψ is the angle between the slip directions of the α th and β th slip systems, ϕ the angle between their slip normals, $\dot{\gamma}^{(\beta)p}$ the plastic strain of the β th slip system, h the strength coefficient, n the work hardening exponent, g the degree of isotropy in work hardening, and ν the thermal softening coefficient. The quantity in the square bracket represents the latent hardening coefficient, and the summation index β ranges over all slip systems. TAYLOR's [1938] isotropic hardening law follows from (15) by setting $g = 1$, and $g = 0$ corresponds to kinematic hardening.

We assume that the plastic slip rates $\dot{\gamma}^{(\alpha)p}$ of all active slip systems at a material point contribute linearly to the plastic parts of the strain rate and spin tensors there through the Schmid factor $\nu_{ij}^{(\alpha)}$ and the antisymmetric part $\omega_{ij}^{(\alpha)}$ of the dyad $\mathbf{b}\mathbf{n}$. Thus,

$$D_{ij}^p = \sum_{\alpha} \nu_{ij}^{(\alpha)} \dot{\gamma}^{(\alpha)p}, \quad W_{ij}^p = \sum_{\alpha} \omega_{ij}^{(\alpha)} \dot{\gamma}^{(\alpha)p}, \quad (16)$$

where

$$\omega_{ij}^{(\alpha)} = \frac{1}{2} (b_i^{(\alpha)} n_j^{(\alpha)} - b_j^{(\alpha)} n_i^{(\alpha)}). \quad (17)$$

The slip direction $\mathbf{b}$ and the unit normal $\mathbf{n}$ to the slip plane are orthogonal unit vectors, and are assumed to rotate with the elastic spin of the lattice. Thus, their rates of change are given by

$$\dot{b}_i = W_{ij}^e b_j, \quad \dot{n}_i = W_{ij}^e n_j. \quad (18)$$

In plane strain deformations of the crystal, the rotation of a slip system can be characterized by the angle change ϕ of the projective direction of the slip vector in the x_1 - x_2 plane. Using eqns (7)₂ and (16)₂ we obtain

$$\dot{\phi} = W_{21}^e = W_{21} - \sum_{\alpha} \omega_{21}^{(\alpha)} \dot{\gamma}^{(\alpha)p}, \quad (19)$$

and rewrite eqns (18) in the form

$$b_1 = \sqrt{1 - b_3^2} \cos \phi_b, \quad b_2 = \sqrt{1 - b_3^2} \sin \phi_b, \quad (20)$$

$$n_1 = \sqrt{1 - n_3^2} \cos \phi_n, \quad n_2 = \sqrt{1 - n_3^2} \sin \phi_n, \quad (21)$$

where ϕ_b and ϕ_n are, respectively, the current angles between the x_1 -axis and the projective directions of the slip vector and the slip plane normal to the x_1 - x_2 plane. They equal the sum of their initial values and their changes with respect to the rotated lattice.

Scaling stress-like quantities by τ_0 , mass density by ρ_0 , length by H , time by H/v_0 , and the temperature by θ_r , we rewrite the above equations in terms of nondimensional variables, and obtain the following.

$$\dot{\rho} + \rho v_{i,i} = 0, \quad (22)$$

$$\delta \rho \dot{v}_i = \sigma_{ij,j}, \quad (23)$$

$$\rho \dot{\theta} = \beta \theta_{,ii} + \sigma_{ij} \sum_{\alpha} \nu_{ij}^{(\alpha)} \dot{\gamma}^{(\alpha)p} + \sigma_{33} \sum_{\alpha} \nu_{33}^{(\alpha)} \dot{\gamma}^{(\alpha)p}, \quad (24)$$

$$\begin{aligned} \dot{\sigma}_{ij} = & (K - \frac{2}{3}G) D_{kk} \delta_{ij} + 2GD_{ij} \\ & - \sum_{\alpha} (2G \nu_{ij}^{(\alpha)} + \omega_{ik} \sigma_{kj} - \sigma_{ik} \omega_{kj}) \dot{\gamma}^{(\alpha)p} - \sigma_{ik} W_{kj} + W_{ik} \sigma_{kj}, \end{aligned} \quad (25)$$

$$\sigma_{33} = -(\sigma_{11} + \sigma_{22}) - 3K \ln \rho, \quad (26)$$

$$\dot{\phi} = W_{21} - \sum_{\alpha} \omega_{21}^{(\alpha)} \dot{\gamma}^{(\alpha)p}, \quad (27)$$

$$\dot{\gamma}^{(\alpha)p} = \begin{cases} \dot{\gamma}_0^{(\alpha)} \left[\frac{(\alpha)}{\tau} \right] \left[\frac{(\alpha)}{\tau_c} \right]^{1/m-1}, & \tau \geq \tau_c, \\ 0, & \tau < \tau_c, \end{cases} \quad (28)$$

$$\tau_c^{(\alpha)} = \left\{ 1 + \sum_{\beta} [g + (1 - g) \cos \psi \cos \phi] h^{(\beta)p} n^{(\beta)} \right\} (1 - \nu \theta) \quad (29)$$

where the nondimensional variables have been denoted by the same symbols as before. Henceforth we will use nondimensional variables only. We note that $2H$ equals the

height of the block, v_0 the steady value of the vertical component of velocity imposed on the top and bottom surfaces, ρ_0 is the mass density in the undeformed and unstressed configuration of the single crystal, and

$$\theta_r = \frac{\tau_0}{\rho_0 c}, \quad \delta = \frac{\rho_0 v_0^2}{\tau_0}. \quad (30)$$

Furthermore, K and G equal, respectively, the bulk and shear moduli of the single crystal.

As pointed out earlier, because of the presumed symmetry of deformations about the horizontal and vertical centroidal axes, we study deformations of the material in the first quadrant. Hence, boundary conditions that follow from the symmetry of deformations are applied on the left and bottom surfaces. Both the top and the right surfaces are taken to be thermally insulated, the right surface is taken to be traction free, and on the top surface zero tangential tractions and a vertical component v_2 of velocity given by

$$-v_2(t) = \begin{cases} t/0.005, & 0 \leq t \leq 0.005, \\ 1, & t \geq 0.005, \end{cases} \quad (31)$$

are prescribed. For the initial conditions, we take

$$\begin{aligned} \rho(\mathbf{x}, 0) &= 1.0, & \mathbf{v}(\mathbf{x}, 0) &= \mathbf{0}, & \boldsymbol{\sigma}(\mathbf{x}, 0) &= \mathbf{0}, \\ \phi(\mathbf{x}, 0) &= 0, & \theta(\mathbf{x}, 0) &= \begin{cases} \epsilon(1 - r^2)^9 \exp(-5r^2), & r \leq 1, \\ 0, & r > 1, \end{cases} \end{aligned} \quad (32)$$

where $r^2 = x_1^2 + x_2^2$. The initially nonuniform temperature field represents a possible imperfection in the single crystal and serves as a triggering mechanism for the localization of the deformation.

III. NUMERICAL SOLUTION AND RESULTS

The problem as formulated above is highly nonlinear and almost impossible to solve analytically. We seek its approximate solution by the finite element method. Equations (22) through (25) and (27) are reduced to a set of coupled nonlinear ordinary differential equations by using the Galerkin approximation (e.g., see HUGHES [1987]) and the lumped mass matrix obtained by assigning one-fourth of the mass of each element to each one of its four nodes. At each node, the mass density, two components of the velocity, temperature, three components σ_{11} , σ_{22} , and σ_{12} of the Cauchy stress, and the angle ϕ characterizing the rotation of the slip system are taken as unknowns. Thus, the number of nonlinear ordinary differential equations equals eight times the number of nodes. The coordinates of nodes are updated after each time increment. Therefore, the spatial domain occupied by the body and the shapes of these elements varies with time. The coupled nonlinear ordinary differential equations are integrated by using the backward-difference Adams method included in the subroutine LSODE taken from the package ODEPACK developed by HINDMARSH [1983], and set $ATOL = 10^{-3}$, $RTOL = 10^{-3}$. The subroutine adjusts the time step adaptively until a solution of the coupled nonlinear ordinary differential equations has been computed to the specified accuracy.

From the computed solution we evaluated $\tau^{(\alpha)}$, $\dot{\gamma}^{(p)}$, $D_{ij}^{(p)}$, and $W_{ij}^{(p)}$ at each quadrature point, and found the plastic slip strain of the active slip system by using

$$\dot{\gamma}^{(p)}(t + \Delta t) = \dot{\gamma}^{(p)}(t) + \Delta t [\dot{\gamma}^{(p)}(t) + \dot{\gamma}^{(p)}(t + \Delta t)]/2.$$

The finite element code developed earlier by BATRA and LIU [1989] to analyze the initiation and growth of shear bands in plane strain compression of the viscoplastic material was modified to study the present problem.

We assigned the following values to various material and geometric parameters in order to compute numerical results.

$$\begin{aligned} k &= 237 \text{ W m}^{-1} \text{ }^{\circ}\text{C}^{-1}, & c &= 960 \text{ J kg}^{-1} \text{ }^{\circ}\text{C}^{-1}, & \rho_0 &= 2700 \text{ kg m}^{-3}, \\ G &= 27.6 \text{ GPa}, & K &= 81.48 \text{ GPa}, & \tau_0 &= 55 \text{ MPa}, & n &= 0.52, \\ h &= 11.02 \text{ MPa}, & m &= 0.02, & \nu &= 0.0222 \text{ }^{\circ}\text{C}^{-1}, & H &= 5 \text{ mm}, \\ g &= 0.28, & v_0 &= 5 \text{ m s}^{-1}, & \epsilon &= 1.0. \end{aligned} \quad (33)$$

Thus, the average applied strain rate equals 1000 s^{-1} , and $\theta_0 = 21.2^{\circ}\text{C}$. The aforestated values are for a typical single crystal of aluminum, except that a rather large value of the thermal softening coefficient ν is used to reduce the CPU time required to initiate a shear band.

An aluminum single crystal has a face-centered-cubic lattice structure, which is characterized by four octahedral slip planes $\{111\}$ and three slip directions $\langle 110 \rangle$ on each plane to give 12 slip systems. Herein all slip systems are assumed to be equally active, and the crystal is compressed along the $[010]$ direction. We study two different cases, namely, when the plane of deformation is parallel to the plane (001) or the plane $(10\bar{1})$ of the single crystal.

We use the maximum principal logarithmic strain ϵ_p , defined as

$$\epsilon_p = \ln \lambda_1 \cong -\ln \lambda_2 \quad (34)$$

to find the deformation at a point. Here λ_1^2 , λ_2^2 , and 1 are eigenvalues of the right Cauchy–Green tensor $C_{\alpha\beta} = x_{i,\alpha} x_{i,\beta}$, or the left Cauchy–Green tensor $B_{ij} = x_{i,\alpha} x_{j,\alpha}$, where $x_{i,\alpha} \equiv \partial x_i / \partial X_\alpha$, X_α being the coordinates of a material point in the stress-free undeformed configuration. The second equality in eqn (34) holds because plastic deformations of the crystal are isochoric, and within the band elastic deformations are minuscule.

We employed a finite element mesh consisting of 32×32 uniform elements in the undeformed configuration, and used 2×2 Gaussian quadrature rule to evaluate various integrals numerically.

III.1. Results when the plane of deformation is parallel to the plane (001) of the single crystal

Figure 1 depicts contours of the maximum principal logarithmic strain ϵ_p for four different values of the average strain, i.e., $\gamma_{\text{avg}} = 0.00355$, 0.02755 , 0.07755 , and 0.10755 . These suggest that a shear band, indicated by higher values of the contours of the maximum principal logarithmic strain near the center, originates at the center and propagates along $\pm 45^{\circ}$ directions and is reflected back from the top surface, with the

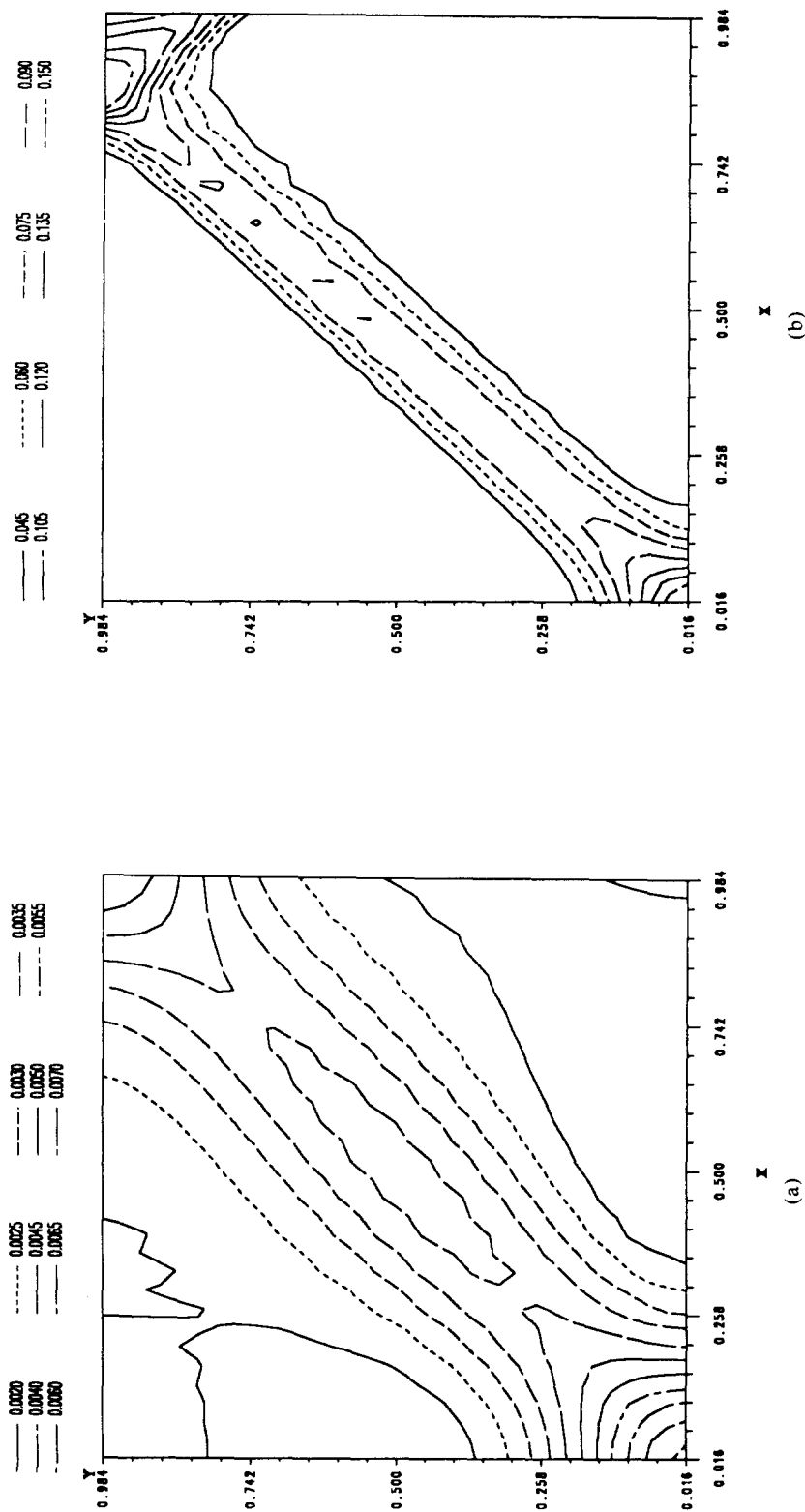


Fig. 1. Contours of the maximum principal logarithmic strain at four different values of the average strain. (a) $\gamma_{avg} = 0.00355$, (b) $\gamma_{avg} = 0.02755$. (Figure continues)

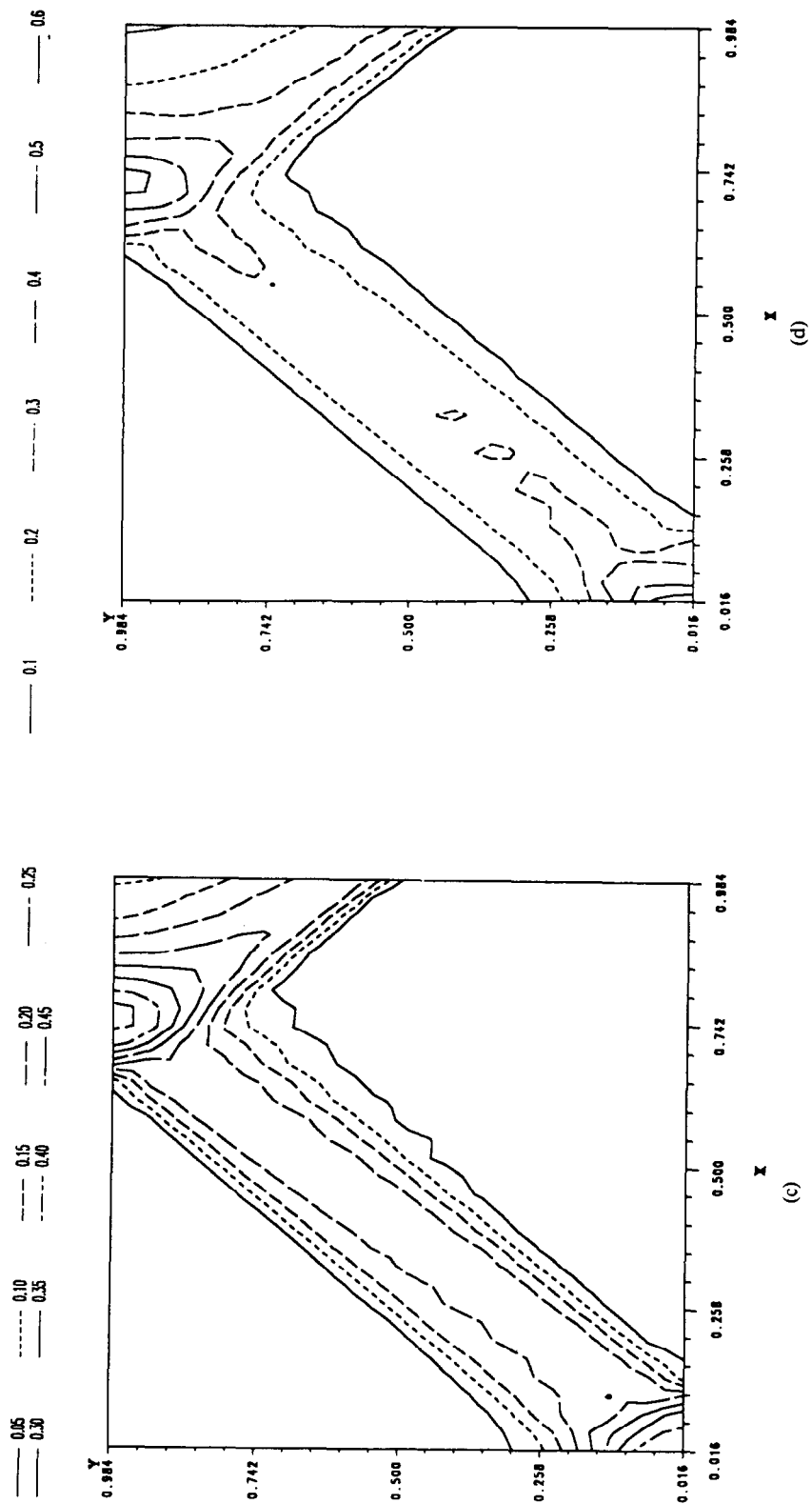


Fig. 1. (c) $\gamma_{\text{avg}} 0.07755$, (d) $\gamma_{\text{avg}} 0.10755$.

angle of reflection being nearly equal to the angle of incidence. The severely deforming region narrows down initially, but then widens, probably because of a change in the locations of the active slip systems. A closer look at the computed results suggests the following. In the beginning, the block is uniformly deformed elastically and all slip systems are inactive in the entire body. As the block continues to be deformed at the high strain rate, the top part of the square cross-section yields first, and the plastic deformation spreads into the body to make four slip systems, namely, $(111)[\bar{1}\bar{1}0]$, $(11\bar{1})[\bar{1}\bar{1}0]$, $(\bar{1}\bar{1}\bar{1})[110]$, and $(\bar{1}\bar{1}\bar{1})[110]$ active. It will be evidenced by results given below. The material surrounding the origin where the temperature perturbation is applied also yields early due to the lower value of the critical shear stress of slip systems at relatively higher temperature. The material adjoining the centroid of the cross-section undergoes more severe plastic deformations than the rest of the material. With further straining of the block, the plastic deformation spreads throughout the body.

The accumulated plastic strain of each active slip system is plotted in Fig. 2 at an average strain of 0.10755. It is clear that four primary slip systems $(111)[\bar{1}\bar{1}0]$, $(11\bar{1})[\bar{1}\bar{1}0]$, $(\bar{1}\bar{1}\bar{1})[110]$, and $(\bar{1}\bar{1}\bar{1})[110]$ contribute significantly to plastic deformations, that the maximum slip strain equals 0.4262, and the average slip strain within the band is approximately 0.175. These slip systems are more favorable to plastic deformation than the slip systems $(111)[0\bar{1}1]$, $(11\bar{1})[0\bar{1}\bar{1}]$, $(\bar{1}\bar{1}\bar{1})[101]$, and $(\bar{1}\bar{1}\bar{1})[10\bar{1}]$ in the central band, and $(\bar{1}\bar{1}\bar{1})[0\bar{1}1]$, $(\bar{1}\bar{1}\bar{1})[011]$, $(111)[10\bar{1}]$, and $(11\bar{1})[101]$ in the reflected band. Note that the average slip strain of the four secondary slip systems in the central band equals 0.025, and that of the slip systems in the reflected band equals 0.01. During the early stages of the shear band formation, only the primary slip systems are active and contribute to the intense plastic deformation within the band. For simple compression in the crystallographic direction $[010]$ and plane of deformation parallel to the crystallographic plane (001) , the four primary slip systems are equally favorable to slip throughout the loading history. However, in a double-slip model for a single crystal employed by ZIKRY and NEMAT-NASSER [1990], the slip system $(111)[\bar{1}01]$, corresponding to $(111)[\bar{1}\bar{1}0]$ in our coordinate system, is chosen as the primary slip system, and $(\bar{1}\bar{1}\bar{1})[011]$ ($(\bar{1}\bar{1}\bar{1})[101]$ in our model) as the conjugate one. These two slip systems are not equally active, with the result that the primary slip system dominates the slip deformation. In our model, all potentially active slip systems are employed, and the slip system becomes active if its resolved shear stress reaches the critical value. The computed results show that all four primary slip systems, namely, $(111)[\bar{1}\bar{1}0]$, $(11\bar{1})[\bar{1}\bar{1}0]$, $(\bar{1}\bar{1}\bar{1})[110]$, and $(\bar{1}\bar{1}\bar{1})[110]$ are equally active. As the single crystal is deformed and the crystal lattice is reoriented by the deformation, other slip systems become active as conjugate slip systems resulting in multiple gliding. The slip systems $(111)[0\bar{1}1]$, $(11\bar{1})[0\bar{1}\bar{1}]$, $(\bar{1}\bar{1}\bar{1})[101]$, and $(\bar{1}\bar{1}\bar{1})[10\bar{1}]$ in the central band, and $(111)[10\bar{1}]$, $(11\bar{1})[101]$, $(\bar{1}\bar{1}\bar{1})[0\bar{1}1]$, and $(\bar{1}\bar{1}\bar{1})[011]$ in the reflected band are the conjugate slip systems.

Figure 3 shows the contours of the slip-rate of the slip system $(111)[\bar{1}\bar{1}0]$ at four different values of the average strain; similar results hold for the other three primary slip systems. At an average strain of 0.00355, the slip rate is nearly uniform throughout most of the single crystal, the only exception being near the block center where temperature perturbation is applied, and near the top right corner where the deformation is singular. With the continuous compression of the block, the region with an intensive slip rate of this system narrows down sharply and the band width equals nearly the smallest distance between two adjacent Gauss points. When compared with the contours of the second invariant of the strain rate and the plastic strain rate tensors given in Fig. 5 below, the slip-rate band of the primary slip systems is aligned in the same direction as the

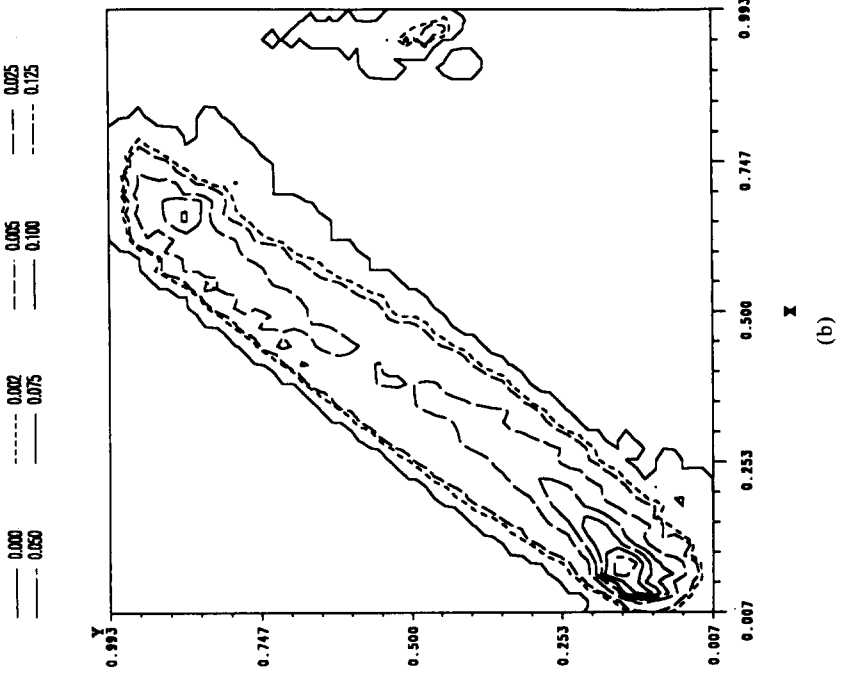
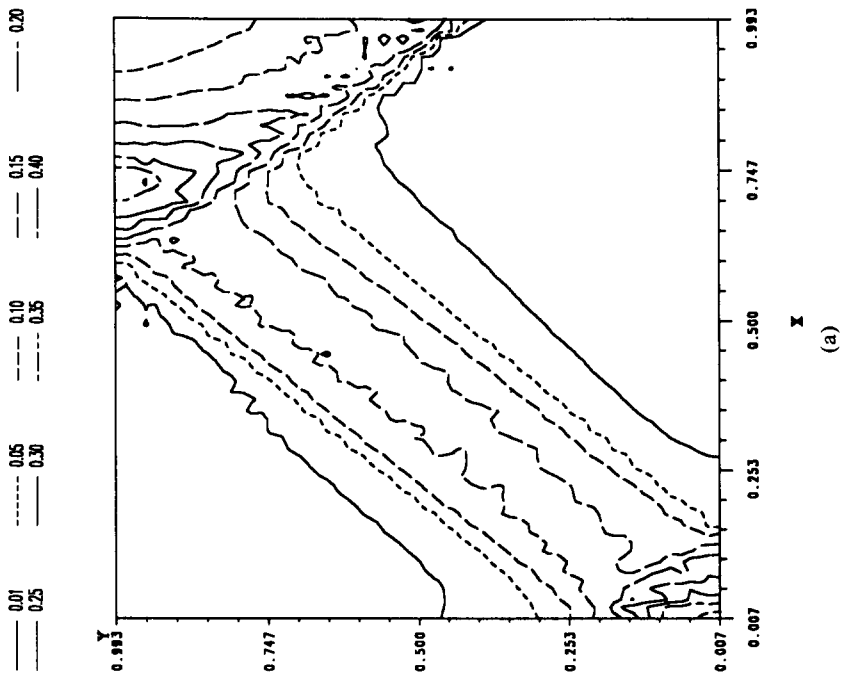


Fig. 2. Contours of the accumulated plastic slip strains of different slip systems at an average strain of 0.10755. (a) Slip systems: $(111)[110]$, $(111)[110]$, and $(111)[110]$, (b) Slip systems: $(111)[011]$ and $(111)[011]$. (Figure continues)

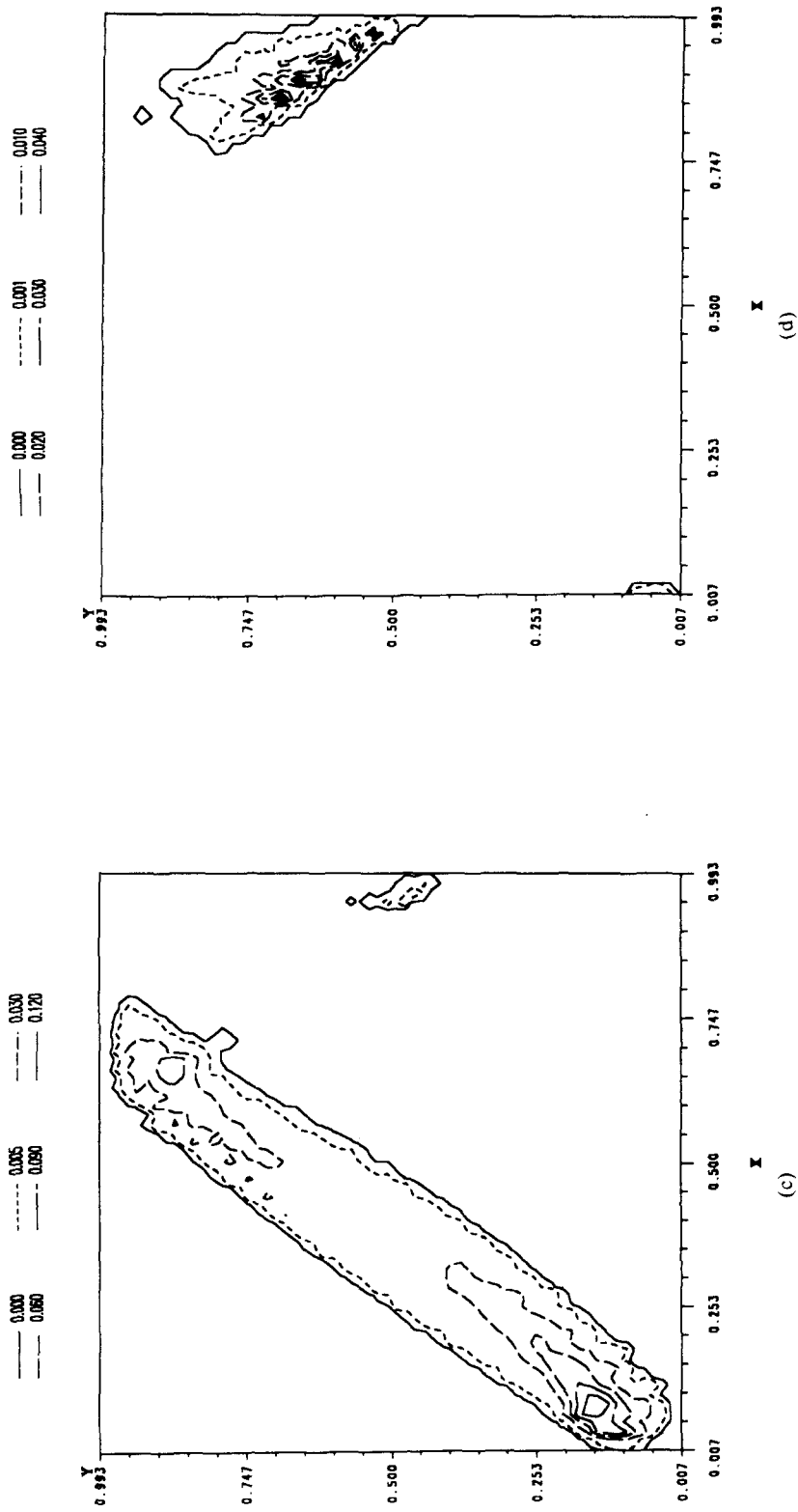


Fig. 2. (c) Slip systems: $(1\bar{1}\bar{1})[101]$ and $(111)[101]$, (d) Slip systems: $(111)[101]$ and $(111)[101]$. (Figure continues)

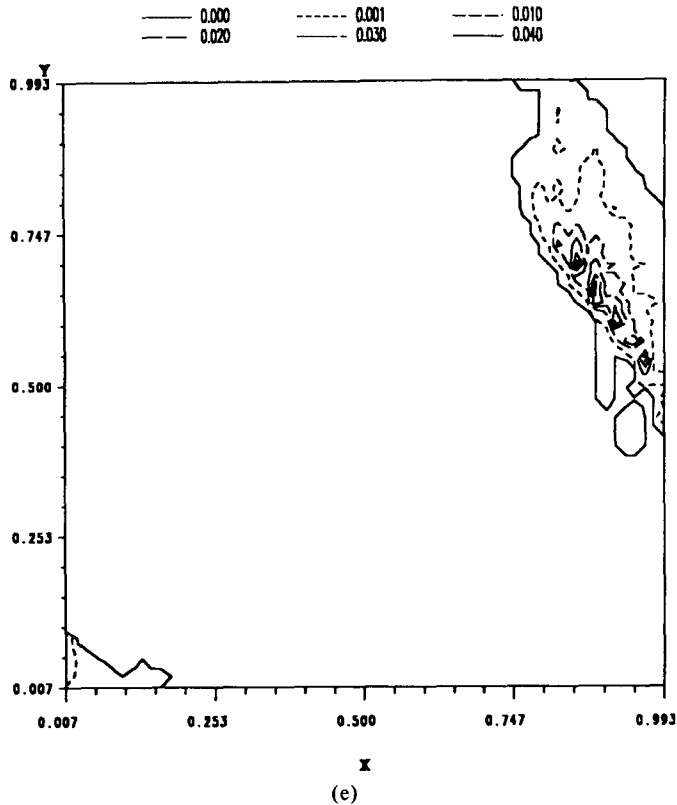


Fig. 2. (e) Slip systems: $(\bar{1}11)[0\bar{1}1]$ and $(1\bar{1}1)[011]$.

global strain-rate band. Note that the double slip model gives a misorientation between the bands of the primary slip system and the global one due to the heterogeneous slip deformations of the primary and the secondary slip systems. An examination of the slip-rate band of the primary slip system at four different values of the average strain suggests that the slip-rate bands broaden as the crystal is deformed. One reason for this widening of the slip-rate band is that once plastic deformation occurs within the slip bands, the work hardening raises the critical shear stress, and further slip deformation in the center of the band may become more difficult than that in the adjacent regions. This facilitates plastic deformation of the material adjacent to the centerline of the slip-rate band. Another reason is that the lattice of the single crystal is reoriented by the deformation, and the widening of the slip-rate band ensures that the centerline of the global band makes an angle of $\pm 45^\circ$ with the direction of the compression loading.

In Fig. 4 we have plotted contours of the slip-rate of slip systems $(111)[0\bar{1}1]$ and $(11\bar{1})[0\bar{1}\bar{1}]$ at average strains of 0.02755, 0.05755, and 0.07755, and that of $(\bar{1}11)[0\bar{1}1]$ and $(1\bar{1}1)[011]$ at average strains of 0.05755 and 0.07755. The slip deformations of slip systems $(1\bar{1}\bar{1})[101]$ and $(1\bar{1}\bar{1})[10\bar{1}]$ are similar to that of $(111)[0\bar{1}1]$. At early stages of deformation, these conjugate slip systems are inactive. Even when the primary slip systems give a severe slip deformation at an average strain of 0.02755, slip systems $(\bar{1}11)[0\bar{1}1]$ and $(1\bar{1}1)[011]$ remain inactive. When the shear bands are fully formed, the

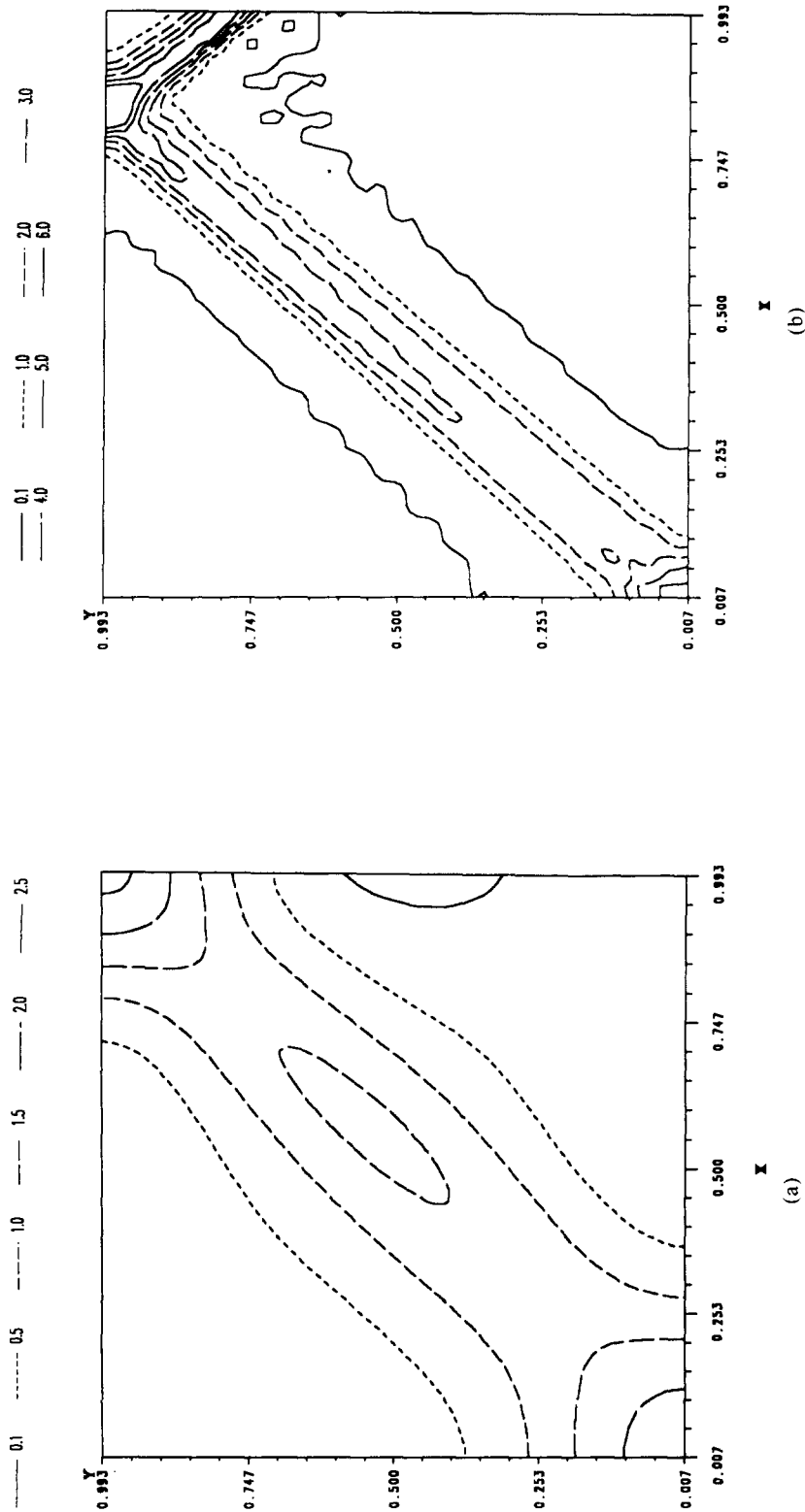


Fig. 3. Contours of the slip-strain-rate of the slip system (111)[100] at four different values of the average strain. (a) $\gamma_{\text{avg}} = 0.00355$, (b) $\gamma_{\text{avg}} = 0.02755$. (Figure continues)

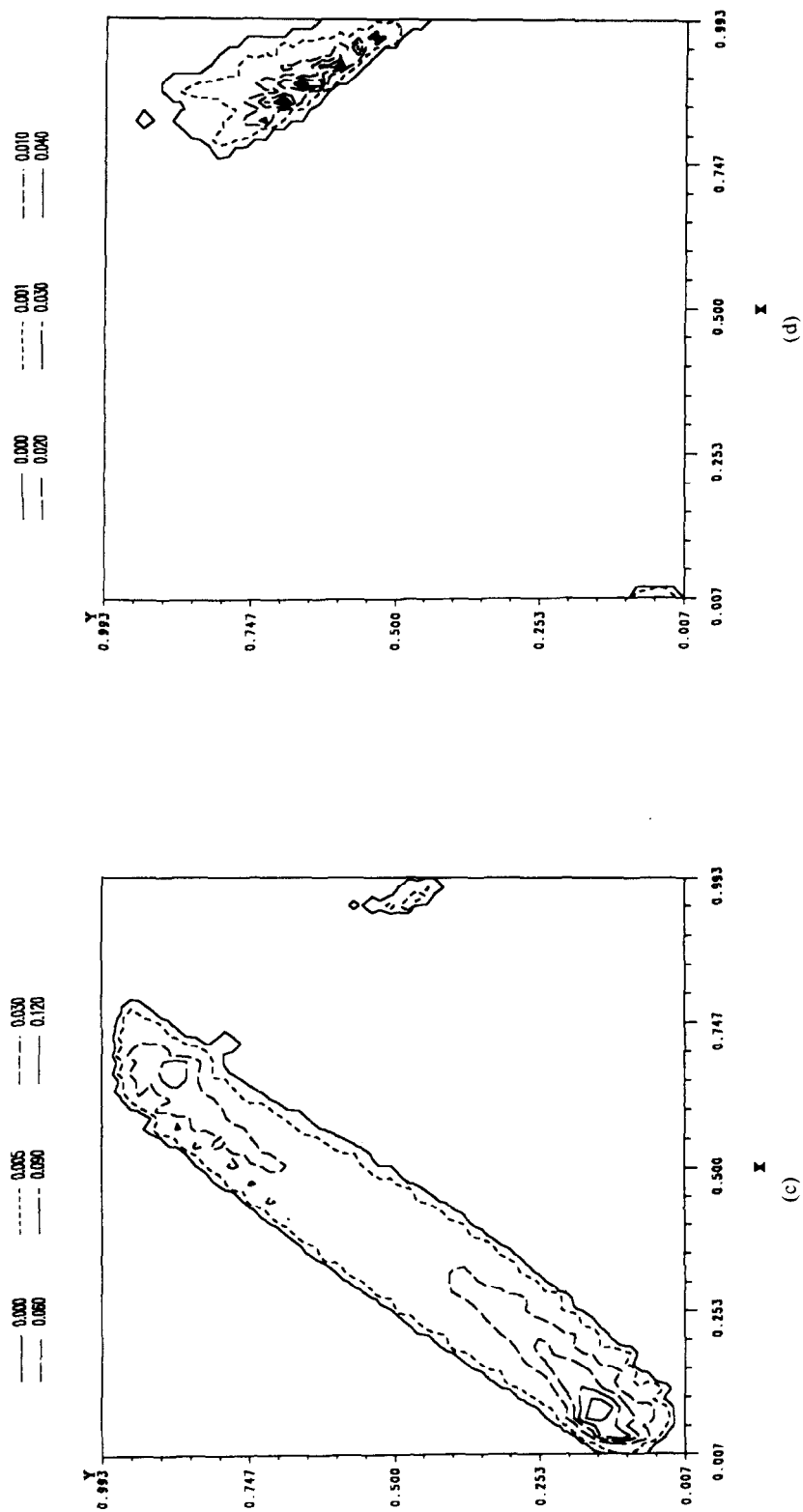


Fig. 2. (c) Slip systems: $(1\bar{1}\bar{1})[101]$ and $(1\bar{1}\bar{1})[101]$, (d) Slip systems: $(1\bar{1}\bar{1})[101]$ and $(1\bar{1}\bar{1})[101]$. (Figure continues)

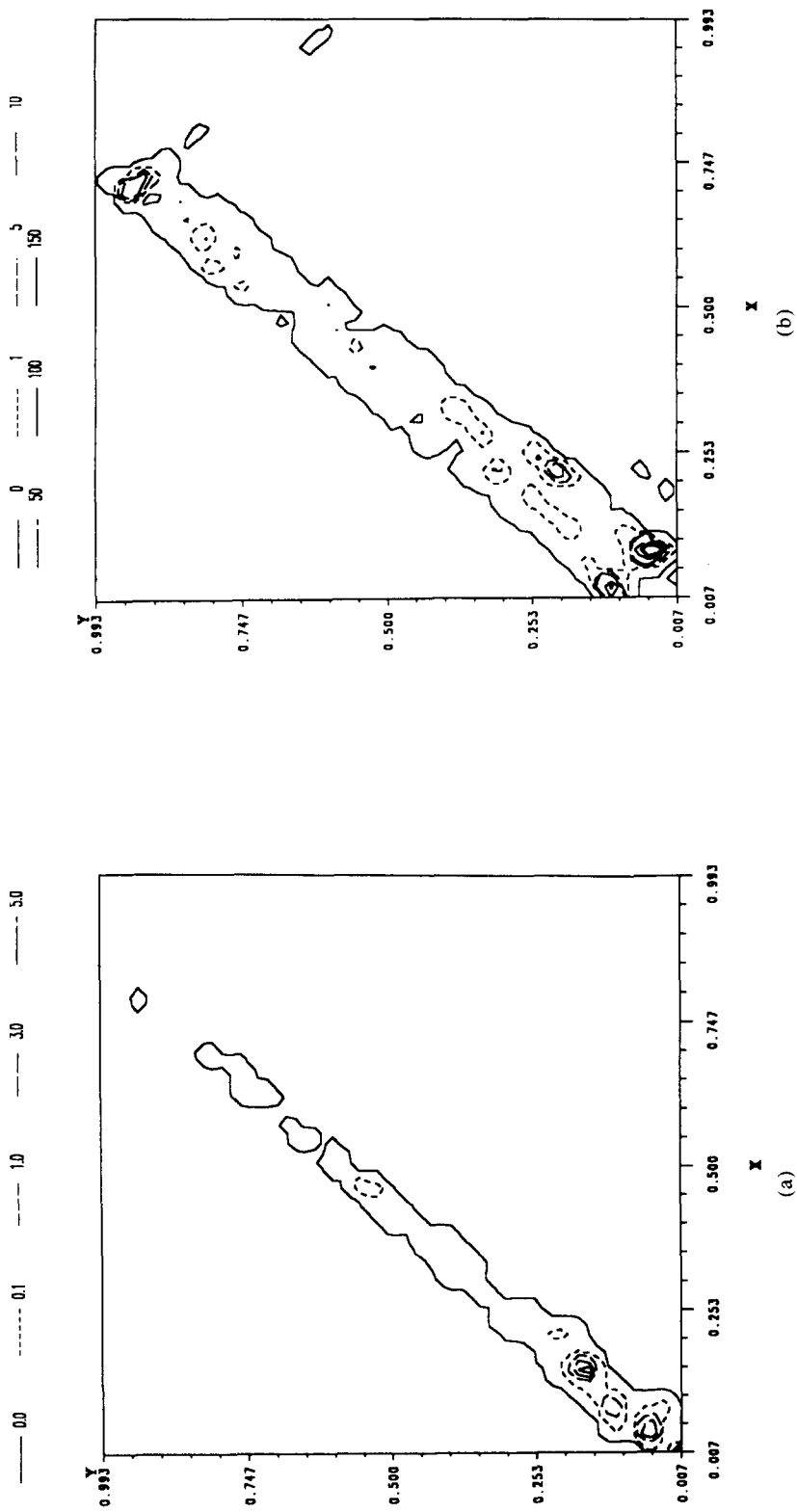


Fig. 4. Contours of the slip-strain-rate of slip systems (111)[011] at (a) $\gamma_{avg} = 0.02755$, (b) $\gamma_{avg} = 0.05755$. (Figure continues)

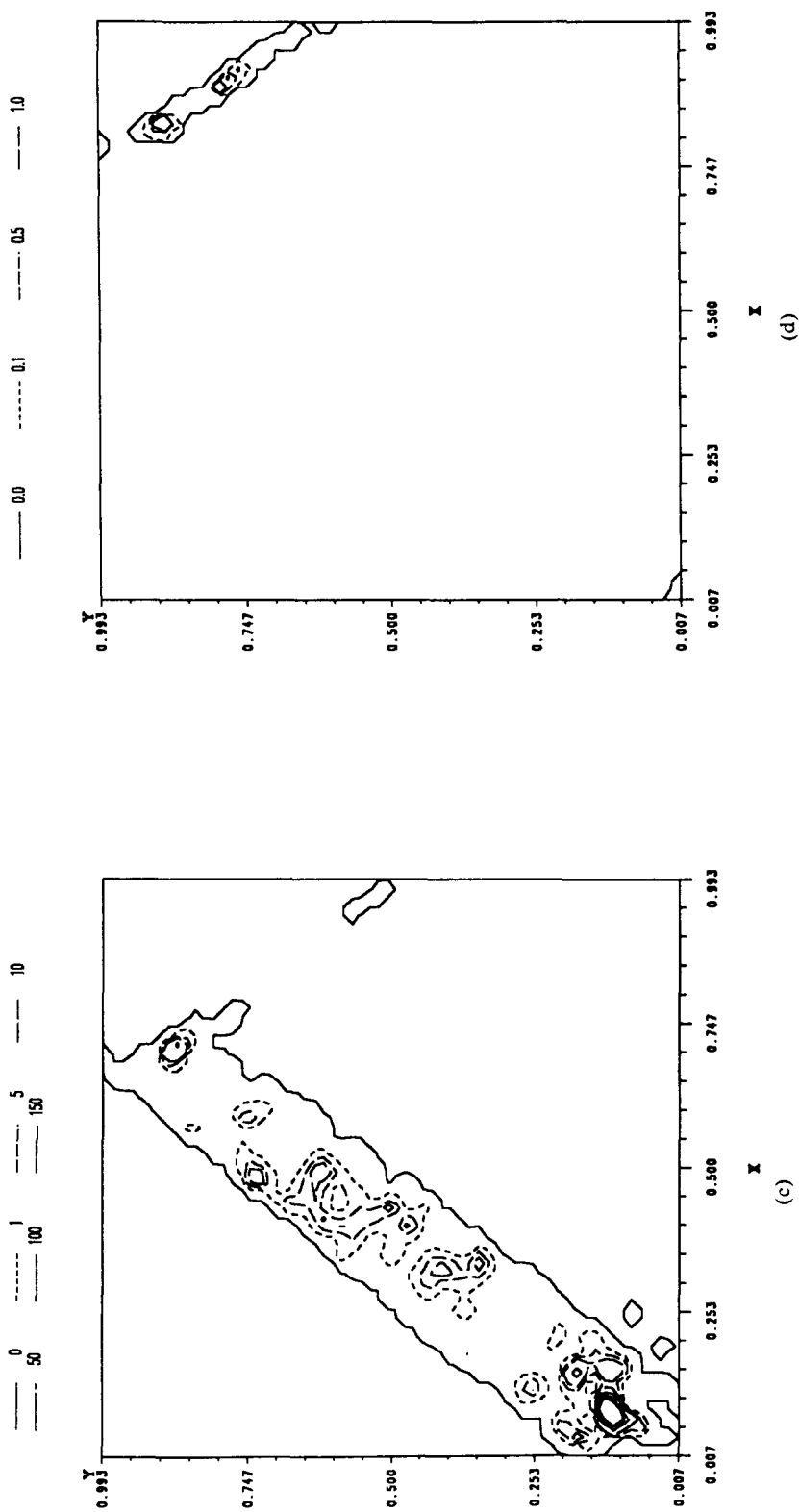


Fig. 4. (c) $\gamma_{\text{avg}} = 0.07755$, and that of slip systems $(\bar{1}11)[0\bar{1}1]$ and $(\bar{1}\bar{1}1)[011]$ and (d) $\gamma_{\text{avg}} = 0.00755$. (Figure continues)

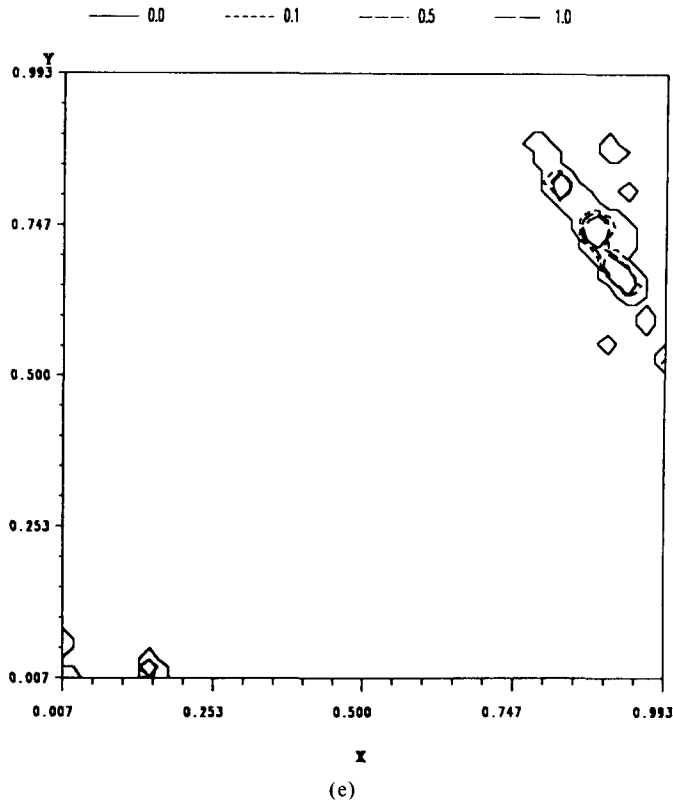


Fig. 4. (e) $\gamma_{\text{avg}} = 0.07755$.

rotation of the crystal lattice relative to the axis of compression results in the movement of the orientation of the stress axis out of its original stereographic triangle into the one adjoining it on the stereographic projection, and the conjugate slip systems become the preferred slip systems.

The contours of the angle of rotation ϕ of the crystal lattice are given in Fig. 5. Within the shear band passing through the block center, the average angle of rotation of slip systems at a nominal strain of 0.00755 is 0.6° counterclockwise, the maximum angle of rotation is 0.726° counterclockwise, and the angle of rotation in the reflected shear band near the top right corner of the block is 0.034° clockwise. However, at a nominal strain of 0.10755, the values of the average and maximum angle of rotation within the central shear band equal, respectively, 14.5° and 18.54° counterclockwise, and those within the reflected band equal 14.3° and 20.3° clockwise.

The contours of the second invariant I of the deviatoric strain-rate tensor $\tilde{D}_{ij}$, and of the second invariant I_p of the plastic strain-rate tensor D_{ij}^p are exhibited in Fig. 6. The invariants I and I_p are defined as

$$2I^2 = \tilde{D}_{ij}\tilde{D}_{ij}, \quad 2I_p^2 = D_{ij}^p D_{ij}^p, \quad \tilde{D}_{ij} = D_{ij} - \frac{1}{3} D_{kk} \delta_{ij}.$$

Recall that $D_{kk}^p = 0$, therefore $\tilde{D}_{ij}^p = D_{ij}^p$. Whereas contours of I or I_p illustrate how rapidly material particles are deforming at present, those of the principal logarithmic strain

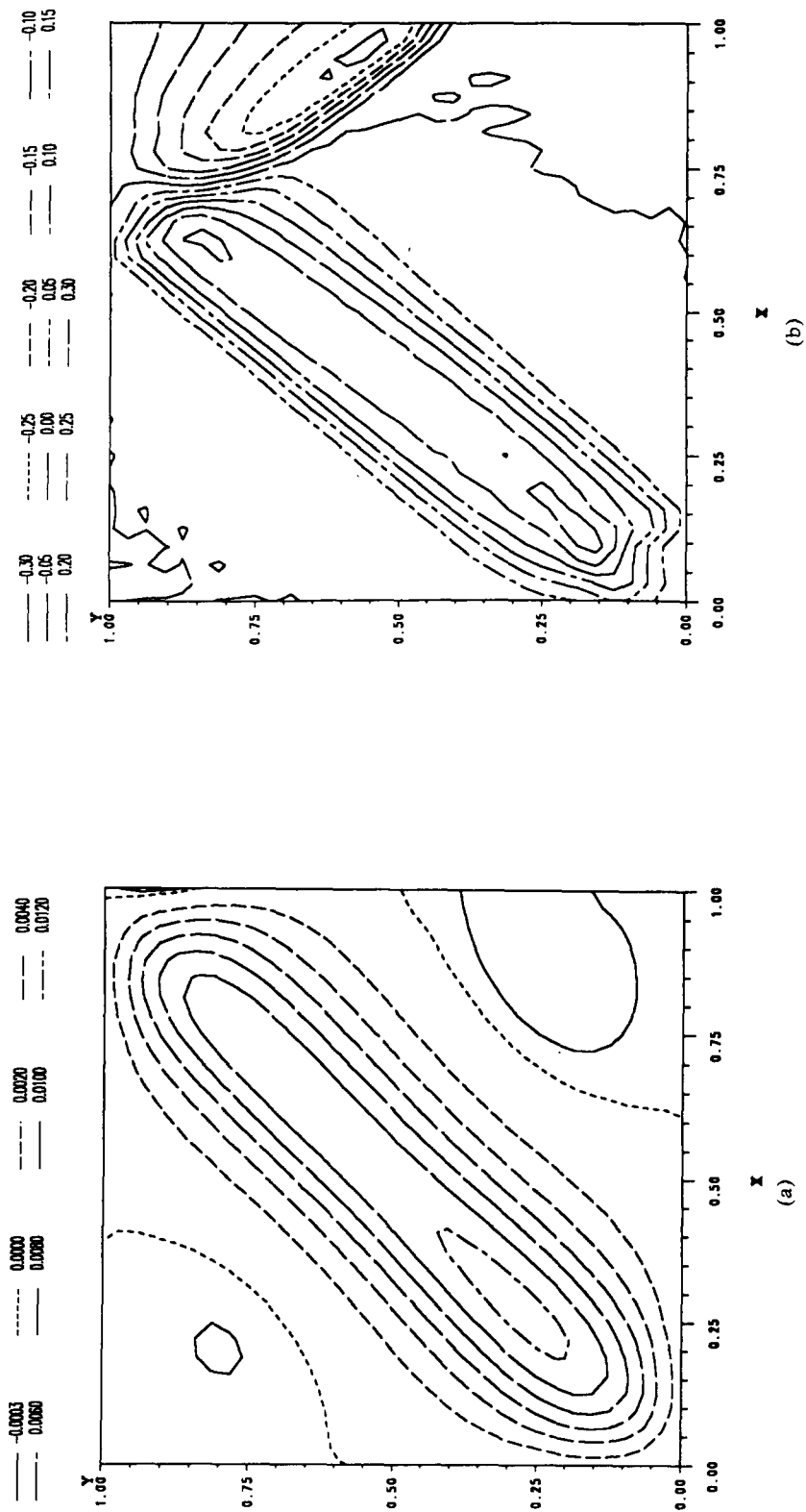


Fig. 5. Contours of the angle of rotation of the crystal lattice at (a) $\gamma_{\text{avg}} = 0.00755$, (b) $\gamma_{\text{avg}} = 0.10755$.

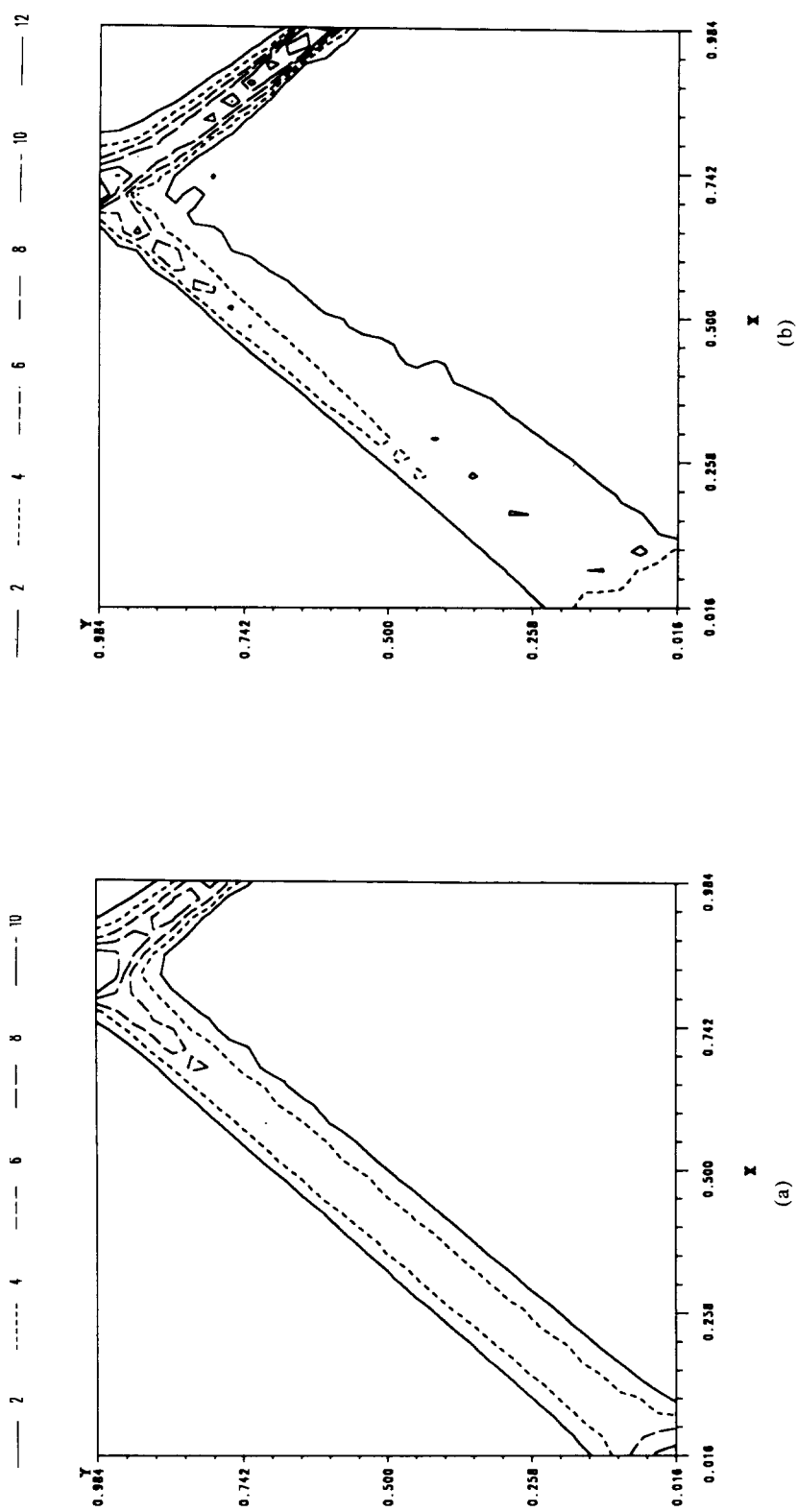


Fig. 6. Contours of the second invariant I of the deviatoric strain-rate tensor at (a) $\gamma_{\text{avg}} = 0.02755$, (b) $\gamma_{\text{avg}} = 0.05755$. (Figure continues)

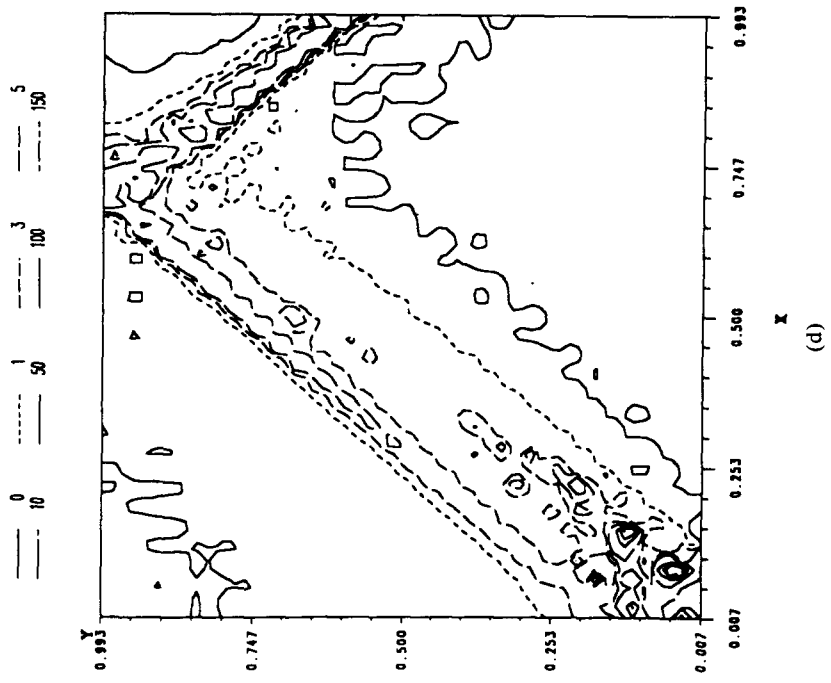
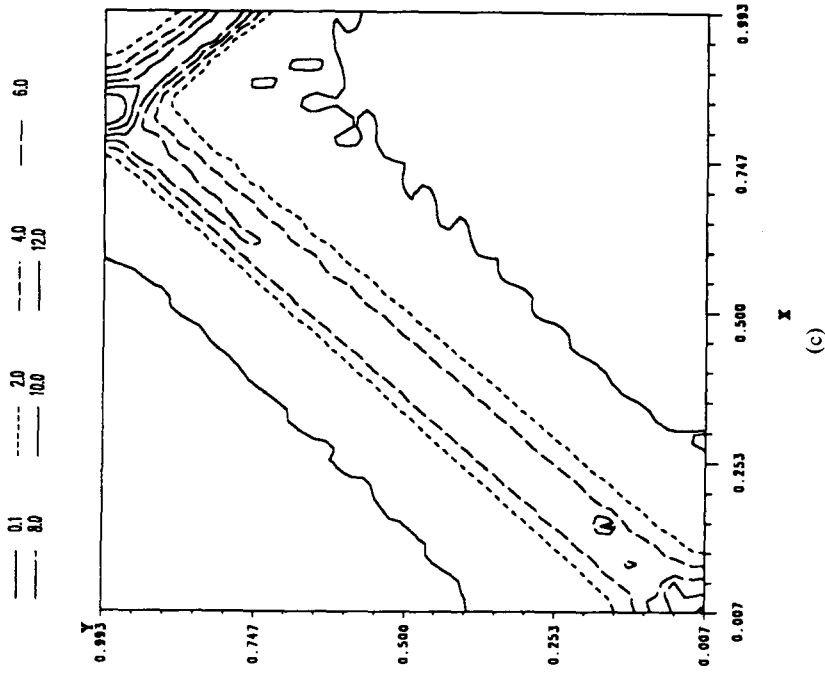


Fig. 6. Contours of the second invariant J_2 of the plastic strain-rate tensor at (c) $\gamma_{avg} = 0.02755$, (d) $\gamma_{avg} = 0.05755$.

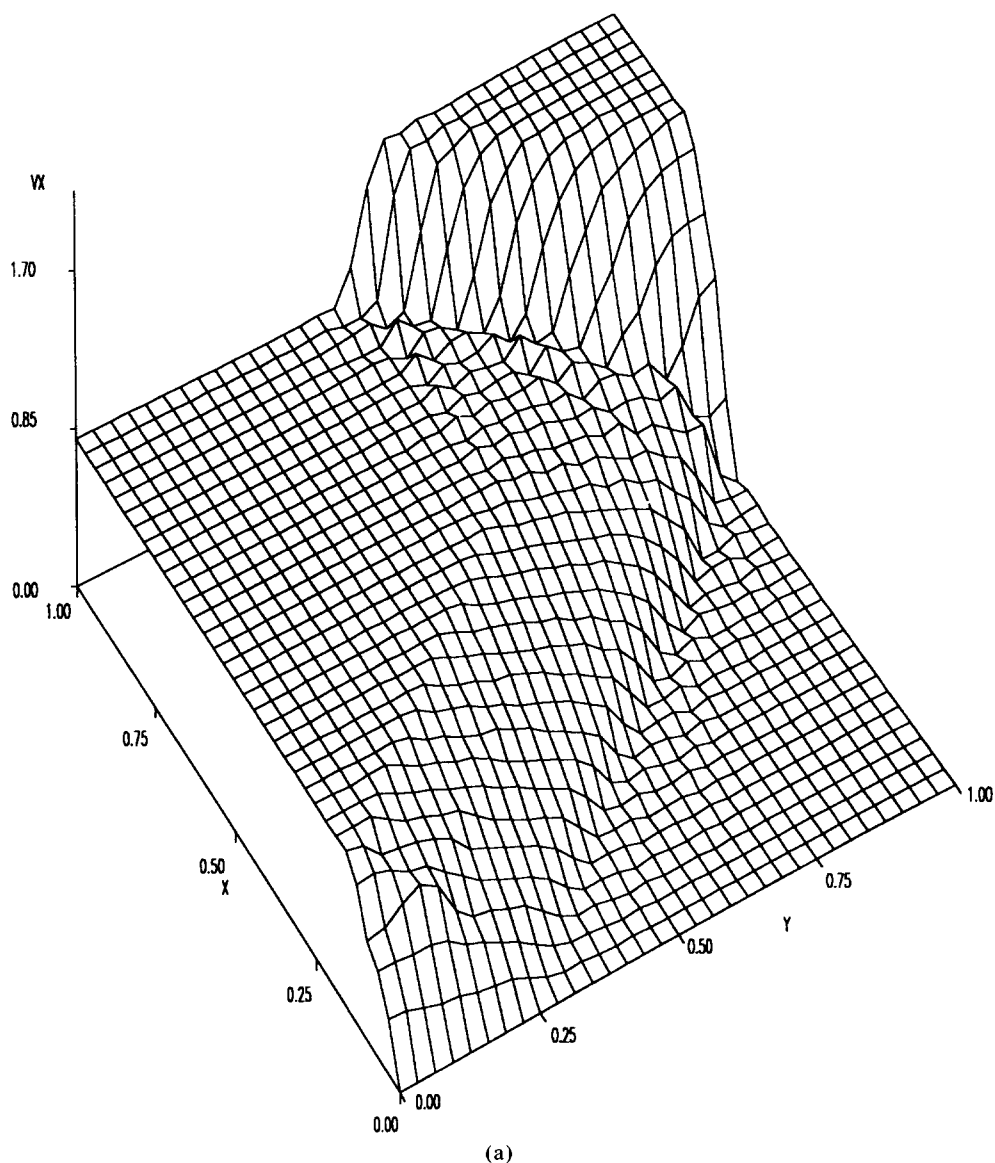


Fig. 7. (a) Distribution of v_x in the cross-section at an average strain of 0.07755. (Figure continues)

given in Fig. 2 correspond to the accumulated deformation of a material element. The values of D_{ij}^p are derived from the plastic straining of the slip systems. At an average strain of 0.02755, the maximum values of I and I_p equal 14.23 and 14.14, respectively, suggesting that the mesh used to calculate nodal values of various variables can delineate the micromechanisms of the slip deformation of active slip systems everywhere. The minimum value 0.00425 of I_p indicates that all of the material particles throughout the cross-section are deforming plastically at $\gamma_{avg} = 0.02755$. However, at an average strain of 0.05755, the maximum values of I_p and I equal 281.84 and 15.43, respectively, and the minimum value of I_p is zero. The contours of I_p in Fig. 6d reveal that the material

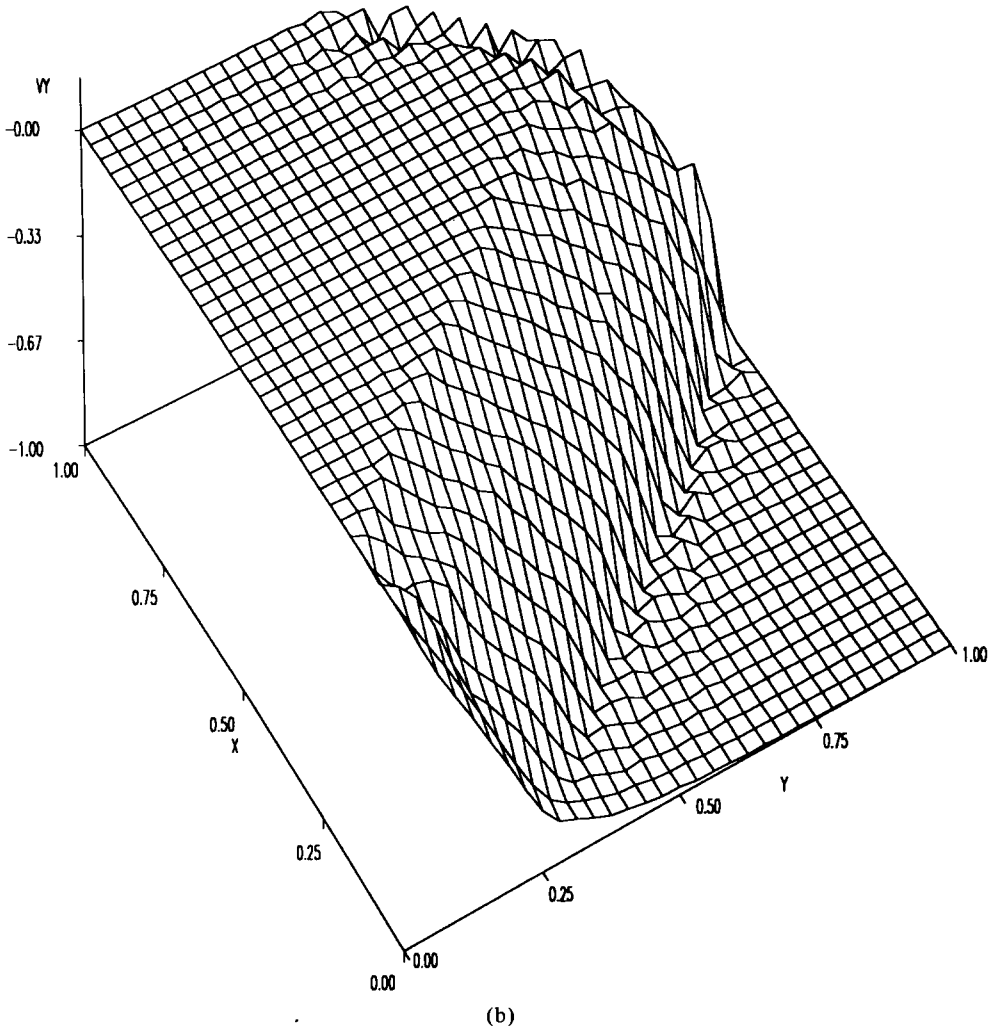


Fig. 7. (b) Distribution of v_y in the cross-section at an average strain of 0.07755.

near the top left and right corners and that near the bottom right corner of the block is deforming elastically, and all slip systems there are inactive. This unloading of the material and possibly the rather coarse mesh used, could cause the significant difference between the maximum values of I and I_p .

Figure 7 depicts the distribution, within the deforming region, of the x - and y -components of the velocity field at an average strain of 0.07755. It is clear that the velocity field increases sharply across the shear band. Note that in our formulation the velocity field is forced to stay continuous throughout the deforming region. Thus, this sharp change in the values of v_x and v_y may be construed as supporting assertions made by TRESCA [1878] and MASSEY [1921] that the tangential component of the velocity field is discontinuous across a shear band.

The deformed mesh at an average strain of 0.11555 is shown in Fig. 8 and confirms the aforementioned observations that a shear band forms along a line passing through the

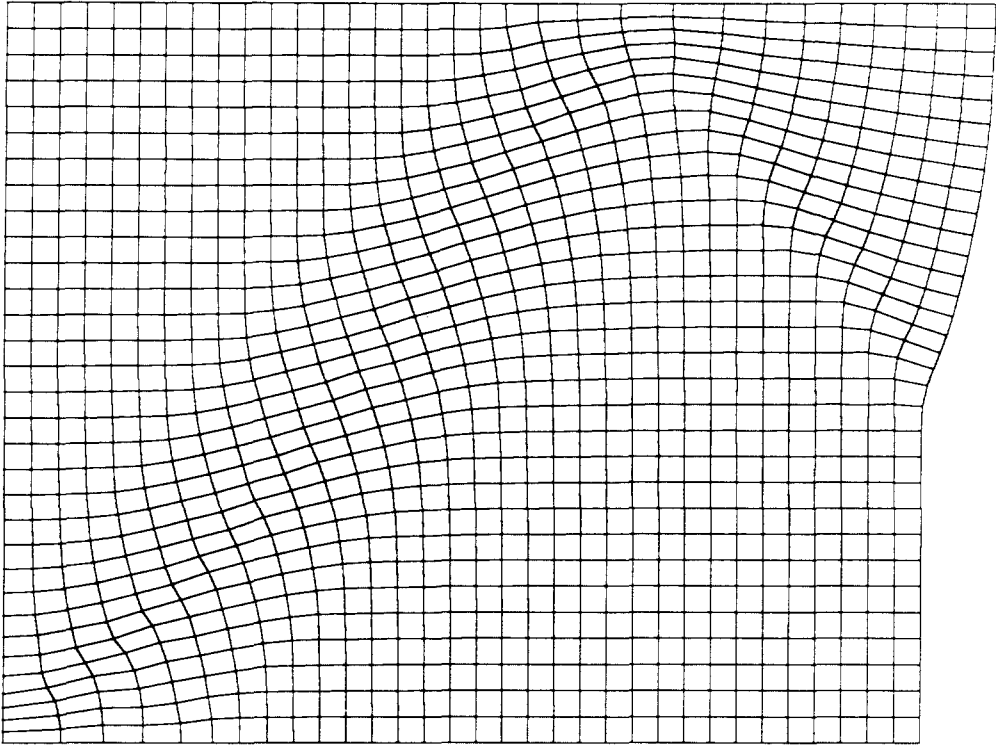


Fig. 8. The deformed mesh at an average strain of 0.11555.

center of the cross-section and making an angle of 45° with the horizontal. The band is reflected from the top surface, and the angle of reflection essentially equals the angle of incidence. The severely deformed region is wider than that obtained in previous computations involving plane strain compression of a homogeneous and isotropic polycrystalline body.

III.2. *The plane of deformation is parallel to the plane $(10\bar{1})$ of the single crystal*

Like the previous case when the plane of deformation is parallel to the plane (001) , the initial plastic deformations of the block are essentially uniformly distributed throughout the cross-section, except near the center where a temperature perturbation is applied. With continuous compression of the block, a shear band initiates from the center and propagates into the body. This is evidenced by the plots, given in Fig. 9, of the contours of the maximum principal logarithmic strain at several values of the average strain. Results plotted in Fig. 9a show that the block is nearly uniformly deformed at an average strain of 0.00255. However, at an average strain of 0.02755, a shear band passing through the center and inclined at an angle of approximately 39.5° with the horizontal has developed. A comparison of this with the results plotted in Fig. 1 suggests that the direction of the shear band in a single crystal depends upon the orientation of the crystal relative to the axis of loading. The contours of the maximum principal logarithmic strain plotted in Figs. 9c and 9d at average strains of 0.07755 and 0.10755 suggest that

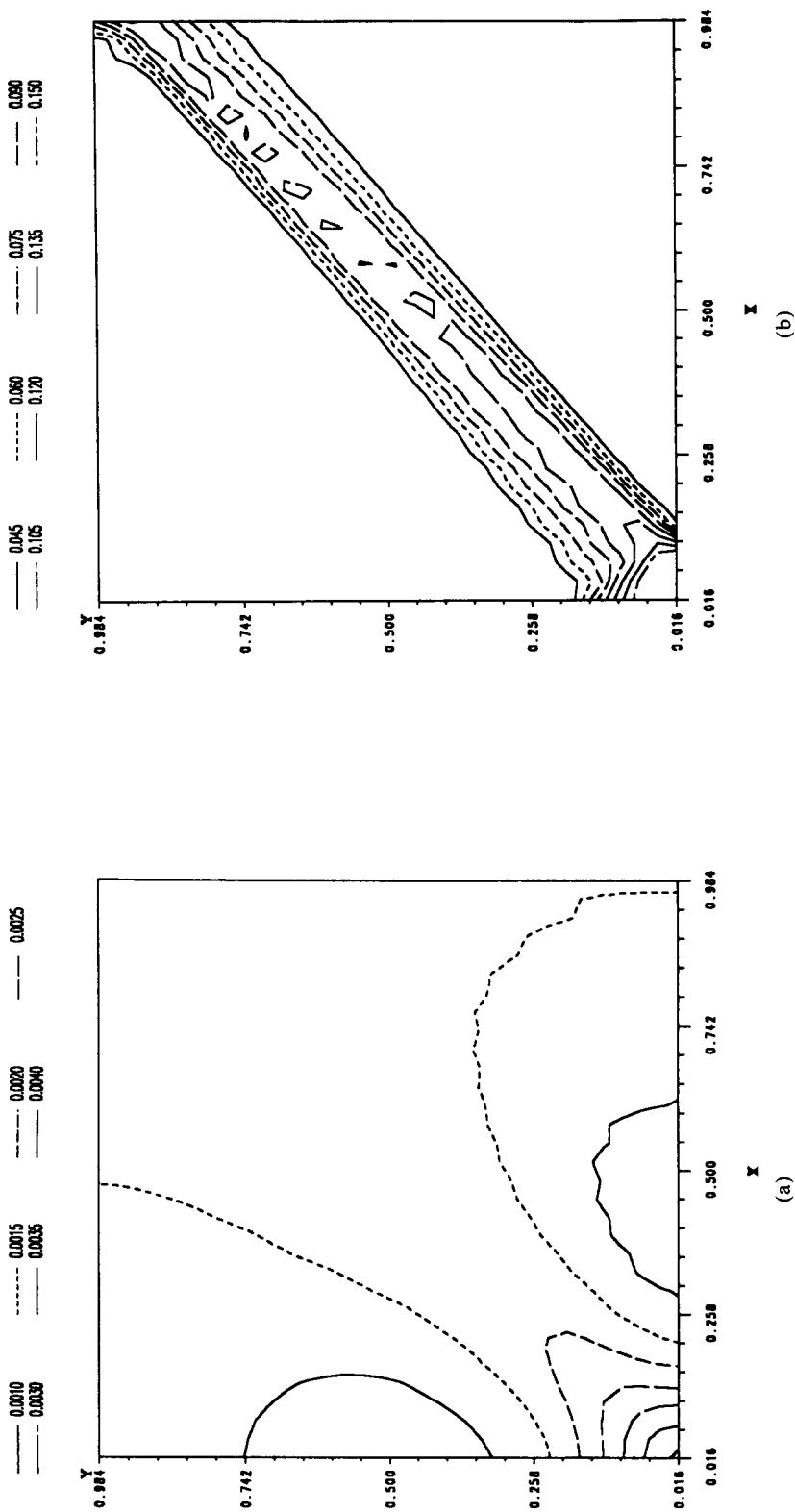


Fig. 9. Contours of the maximum principal logarithmic strain at four different values of the average strain. (a) $\gamma_{\text{avg}} = 0.00255$, (b) $\gamma_{\text{avg}} = 0.02755$. (Figure continues)

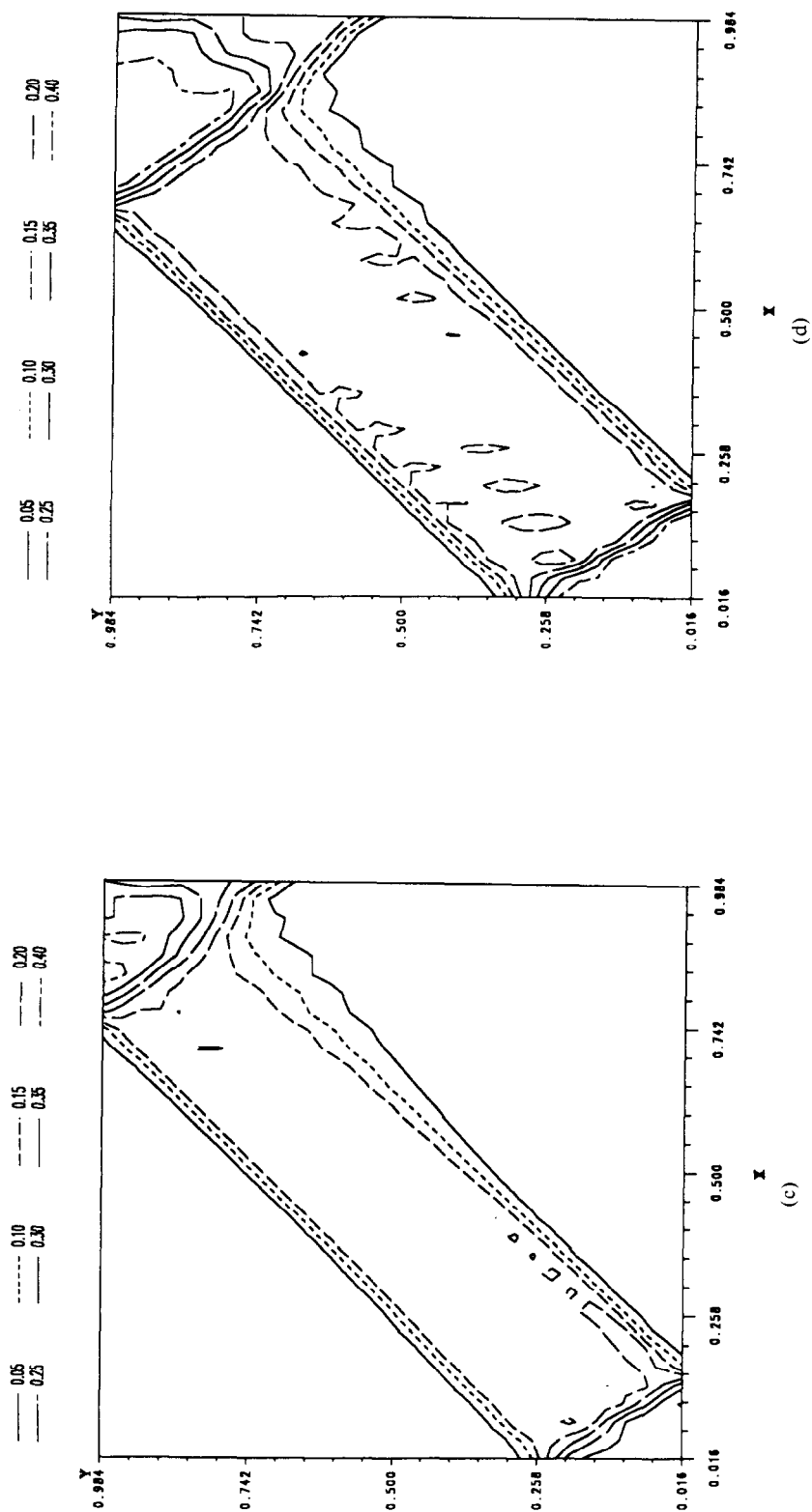


Fig. 9. (c) $\gamma_{avg} = 0.07755$, (d) $\gamma_{avg} = 0.10755$.

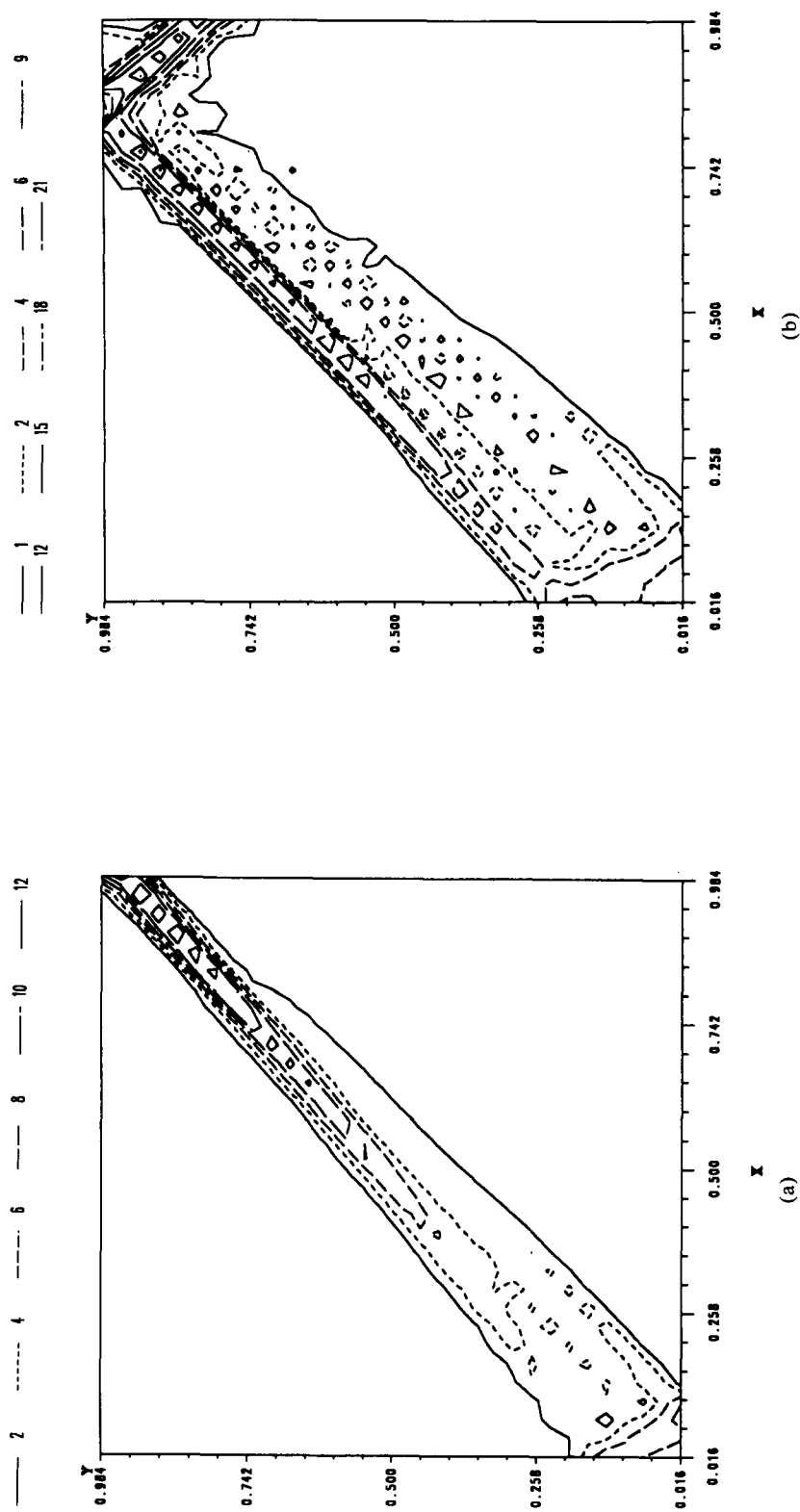


Fig. 10. Contours of the second invariant I of the deviatoric strain-rate tensor at three different values of the average strain. (a) $\gamma_{\text{avg}} = 0.02755$, (b) $\gamma_{\text{avg}} = 0.05755$. (Figure continues)

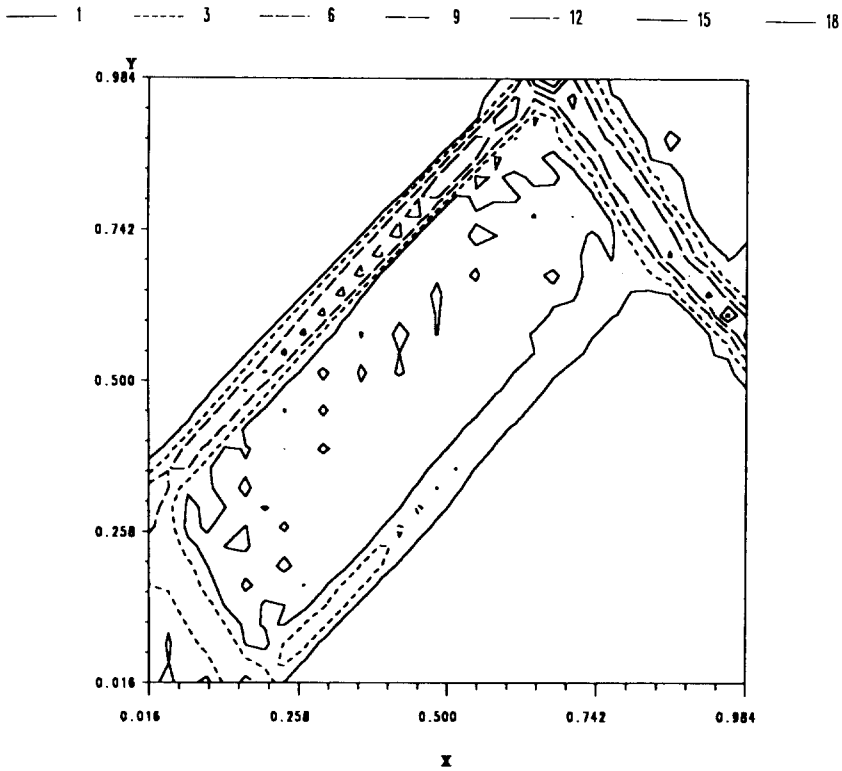


Fig. 10. (c) $\gamma_{\text{avg}} = 0.10755$.

the band widens as the body continues to be compressed, and the width of the severely deformed region is more than that in the previous case discussed in section III.1.

The contours of the second invariant I of the deviatoric strain-rate tensor and of the second invariant I_p of the plastic strain-rate tensor are given in Figs. 10 and 11, respectively. The results plotted in Fig. 10 suggest that initially the band initiating from the centroid of the cross-section meets the right traction free surface. As the band widens, another band reflected from the top surface also forms. With further loading of the body, the band through the center of the cross-section splits into two parallel bands of unequal intensity as measured by the maximum values of I in them; the upper stain-rate band has higher intensity of deformation than the lower one, and is reflected back into the body from the top loading surface. The lower band meets the reflected band and does not go through it, possibly because of the higher values of I in the reflected band. The contours of I_p in Fig. 11d reveal that a large region near the upper left and lower right corners of the cross-section is deforming elastically at an average strain of 0.10755. Since the body continues to be compressed at the prescribed rate, the unloading in regions near the upper left and lower right corners should intensify the rate of plastic deformation elsewhere.

We have plotted in Fig. 12 the angle of rotation of the crystal lattice at several different values of the average strain. At a nominal strain of 0.00755, the maximum and minimum values of the angle of rotation equal 1.47° counterclockwise and 0.08° clockwise. However, at a nominal strain of 0.10755, the average angle of rotation within the

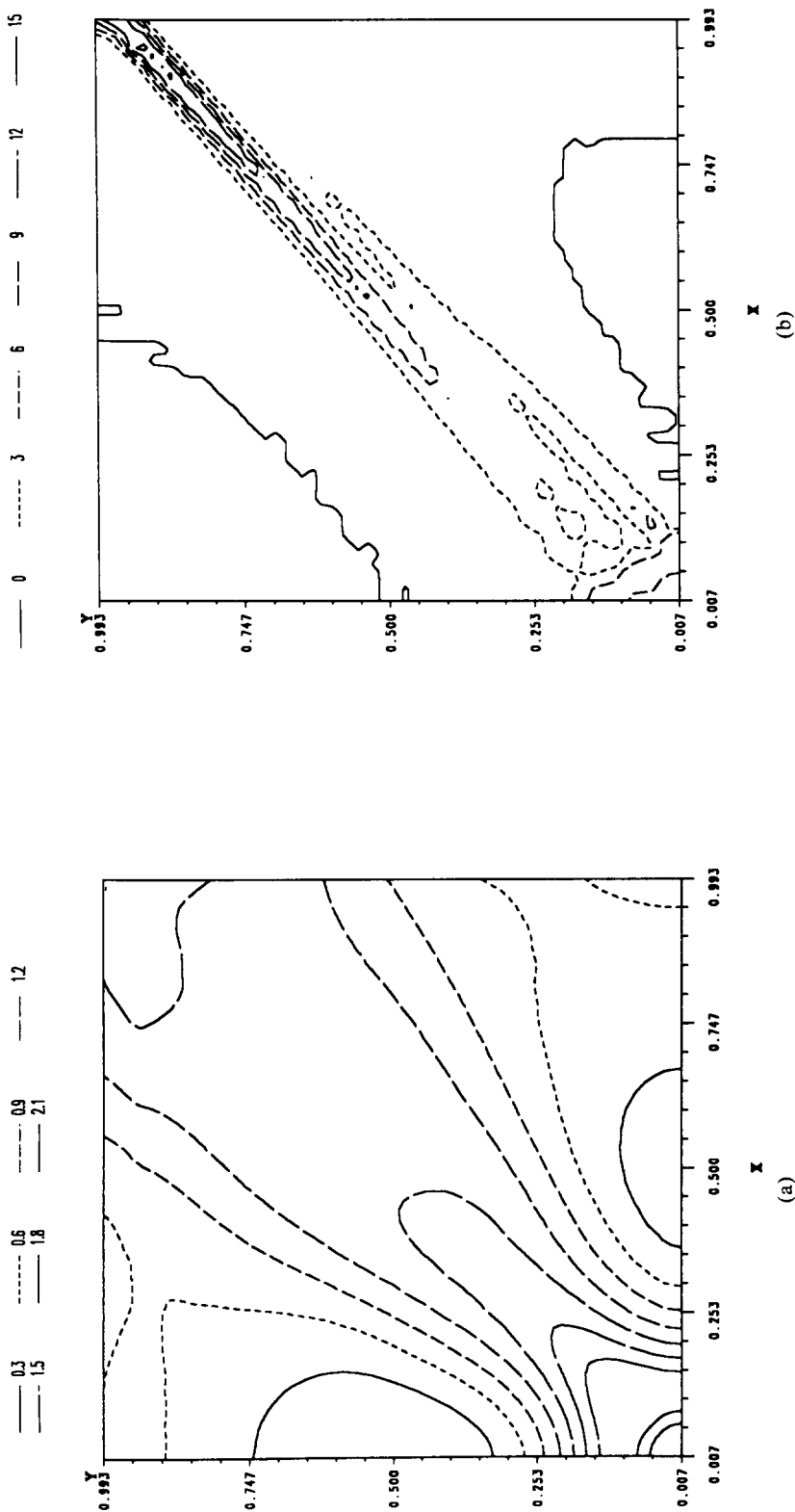


Fig. 11. Contours of the second invariant I_ρ of the plastic strain-rate tensor at four different values of the average strain. (a) $\gamma_{avg} = 0.00255$, (b) $\gamma_{avg} = 0.02755$. (Figure continues)

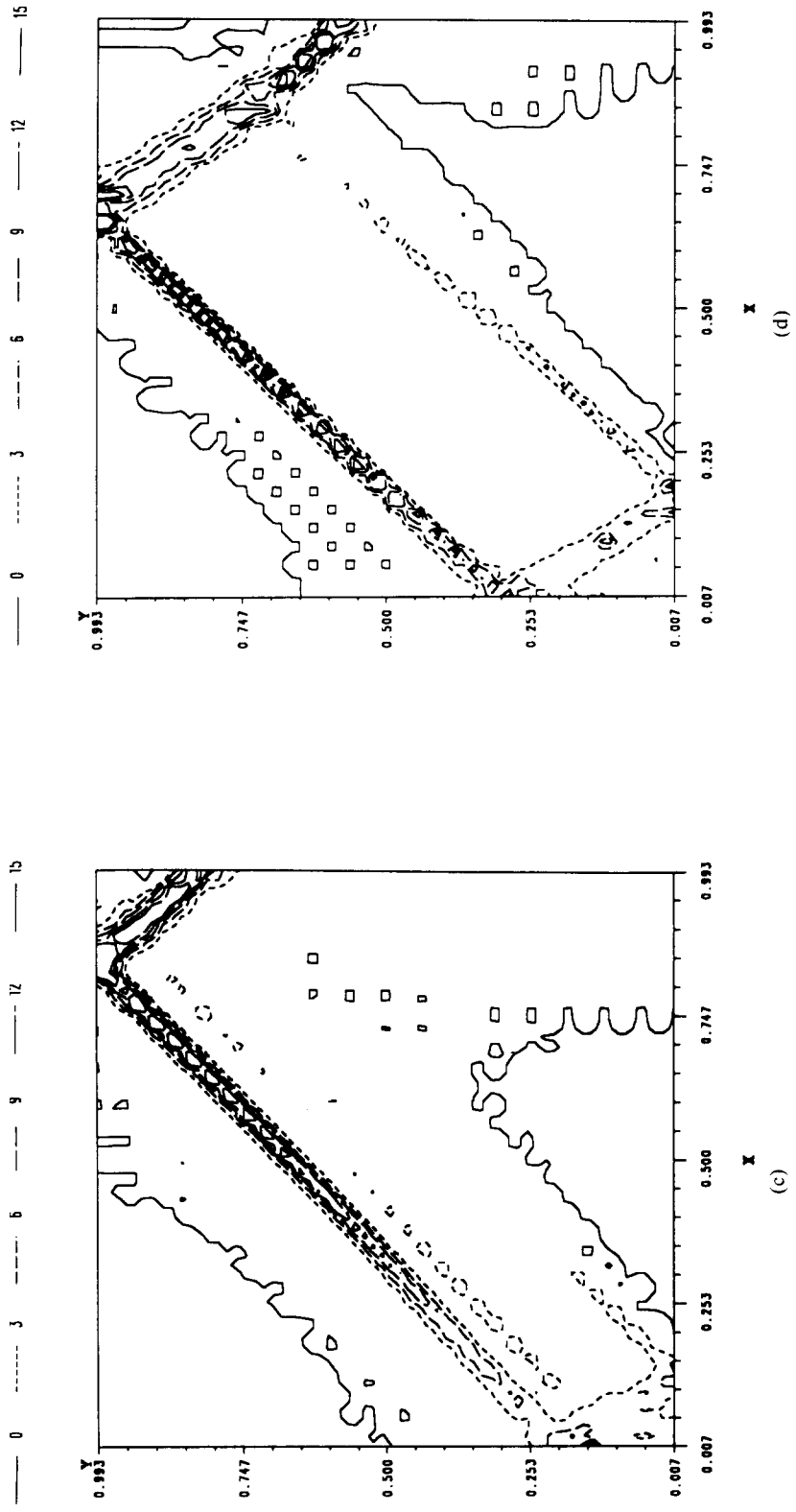


Fig. 11. (c) $\gamma_{\text{avg}} = 0.05755$, (d) $\gamma_{\text{avg}} = 0.10755$.

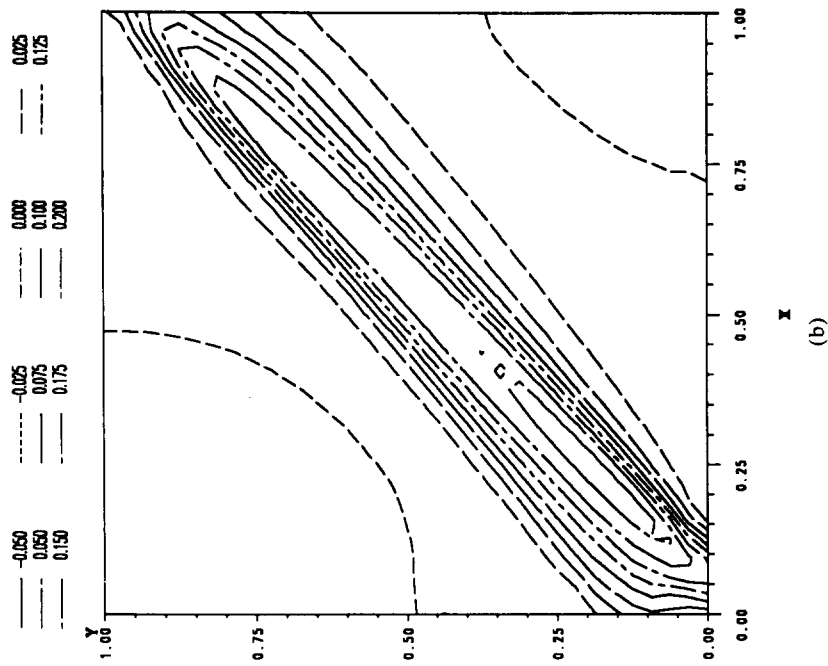
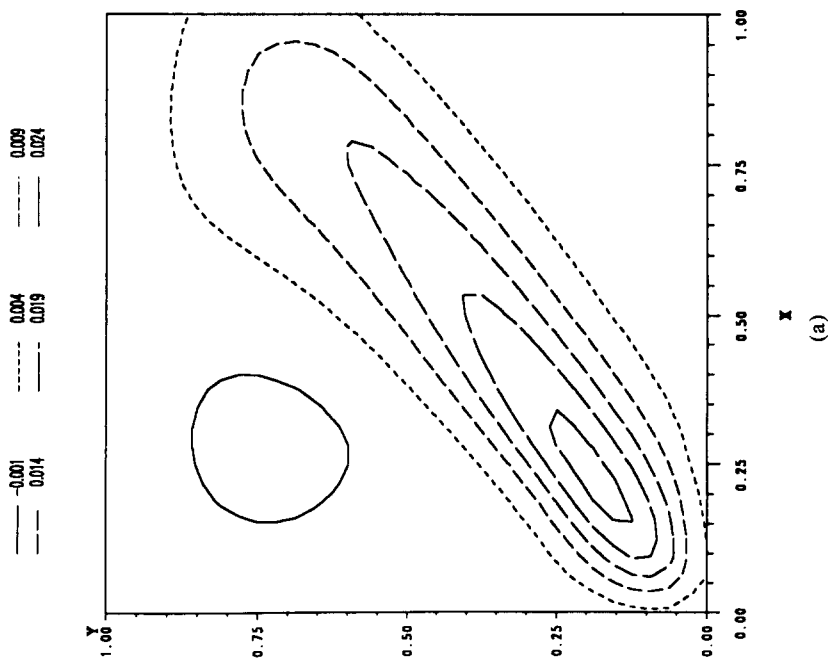


Fig. 12. Contours of the angle of rotation of the crystal lattice at three different values of the average strain. (a) $\gamma_{\text{avg}} = 0.00755$, (b) $\gamma_{\text{avg}} = 0.02755$. (Figure continues)

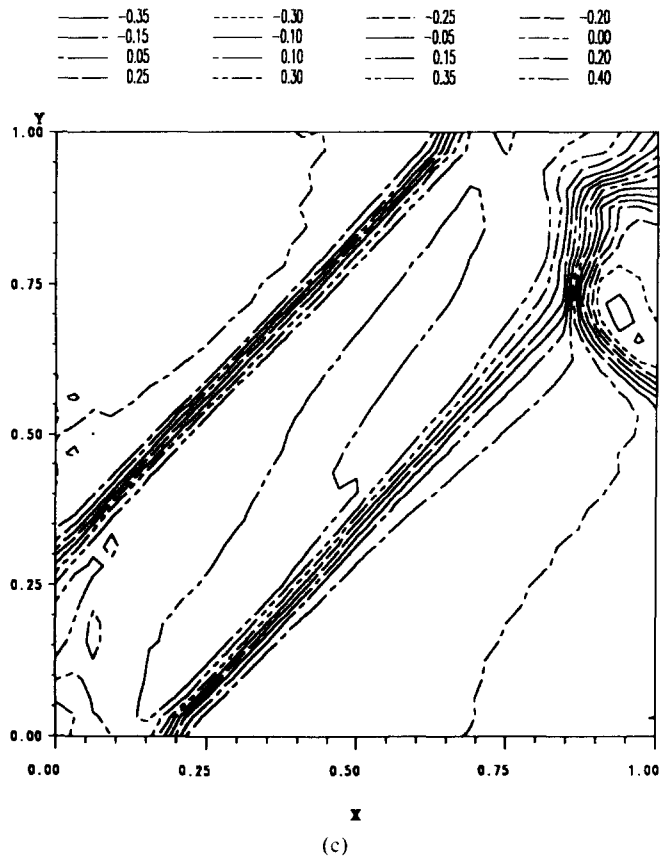


Fig. 12. (c) $\gamma_{\text{avg}} = 0.10755$.

central shear band is 22.9° counterclockwise, and in the reflected band is 17.2° clockwise. These values indicate that the crystal lattice undergoes significant rotations within the shear band.

The distribution of the x - and y -components of the velocity field within the cross-section, at an average strain of 0.0755, is plotted in Figs. 13a and 13b, respectively. It is clear that the deforming region is subdivided into several subregions and the velocity field changes sharply across boundaries between these regions; the changes in v_x and v_y across the upper central band are more than those across the lower central band.

The accumulated slip strains in different slip systems revealed that the slip systems $(111)[10\bar{1}]$ and $(\bar{1}\bar{1}1)[10\bar{1}]$ remained inactive throughout the entire loading history. Slip systems $(111)[1\bar{1}0]$ and $(111)[0\bar{1}1]$ in both the central and the reflected band, and slip systems $(\bar{1}\bar{1}1)[110]$ and $(\bar{1}\bar{1}1)[011]$ in the reflected band were found to be more active than other slip systems. Figures 14 and 15 depict, respectively, the contours of slip strains and slip strain-rates at an average strain of 0.10755. At this value of the nominal strain, the average slip strain of slip systems $(111)[1\bar{1}0]$ and $(111)[0\bar{1}1]$ in the central band equals 0.2 and that in the reflected band is 0.5, and slip systems $(\bar{1}\bar{1}1)[110]$ and $(\bar{1}\bar{1}1)[011]$ have an average slip strain of 0.17 in the reflected band. Other active slip systems give very small values of the slip strains within the bands. From contours of slip strain rates in

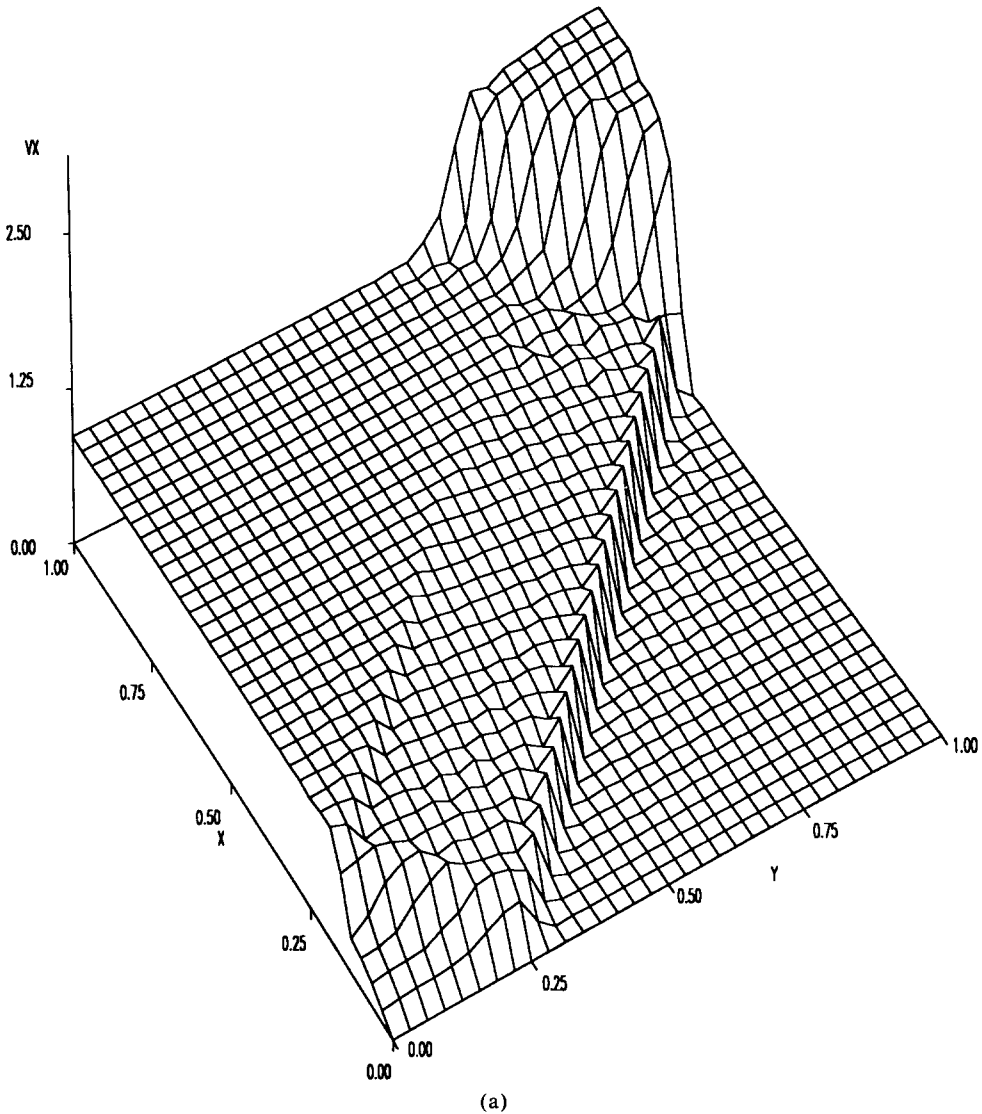


Fig. 13. (a) Distribution of v_x in the cross-section at an average strain of 0.07755.

Fig. 16, we see that at an average strain of 0.00255, only four slip systems, viz., $(111)[\bar{1}\bar{1}0]$, $(111)[0\bar{1}1]$, $(\bar{1}\bar{1}1)[110]$, and $(\bar{1}\bar{1}1)[011]$ are active everywhere in the block. The narrow region with intensive slip-rate deformation for slip systems $(111)[\bar{1}\bar{1}0]$ and $(111)[0\bar{1}1]$ differs from that for slip systems $(\bar{1}\bar{1}1)[110]$ and $(\bar{1}\bar{1}1)[011]$, in contrast with the case discussed in section III.1 wherein all four primary slip systems are equally active in the same narrow region. However, the intensity of slip-rates in the two narrow regions seems to be nearly the same. Since, in simple compression, the slip systems $(111)[\bar{1}\bar{1}0]$ and $(111)[0\bar{1}1]$ are more favorable to slip than the other two primary slip systems, these two slip systems eventually dominate the slip deformation of the single crystal and the slip systems $(\bar{1}\bar{1}1)[110]$ and $(\bar{1}\bar{1}1)[011]$ become inactive in the central bands.

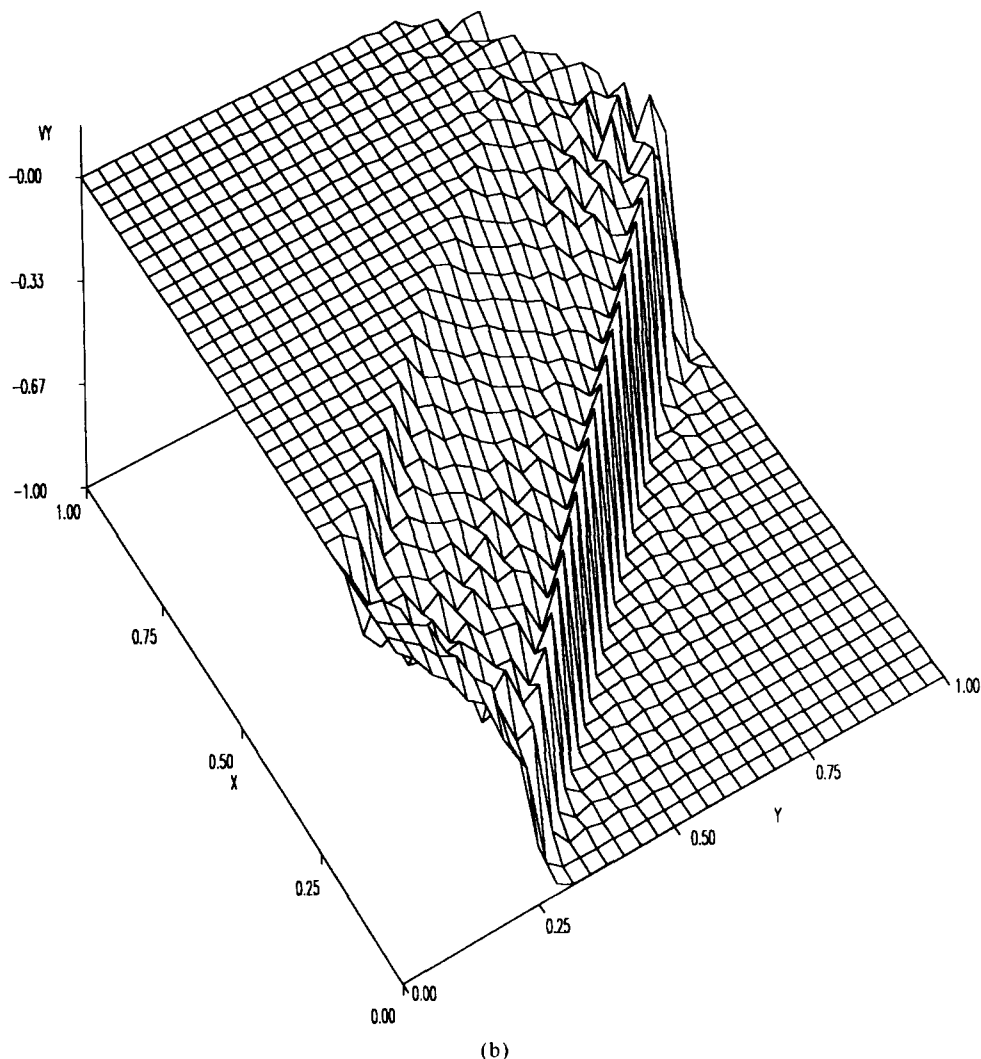


Fig. 13. (b) Distribution of v_y in the cross-section at an average strain of 0.07755.

Figure 17 exhibits the average axial stress versus the average axial strain for the two loading cases studied herein. The average axial stress is obtained by evaluating σ_{22} at quadrature points closest to the top surface of the block and taking their average. The average axial strain equals the vertical displacement of the top surface divided by the initial height of the specimen. In the figure compressive axial stress and compressive axial strain are plotted as positive. For the second loading case, the curve corresponding to the initial loading of the block is missing because of the loss of a part of the output from the computer code. For each loading case, the transient effects die out quickly, and the average axial stress decreases monotonically with an increase in the average strain because the softening of the material caused by its being heated up exceeds the combined hardening due to strain and strain-rate effects. It is due to the rather large value of the thermal softening coefficient assumed in our work.

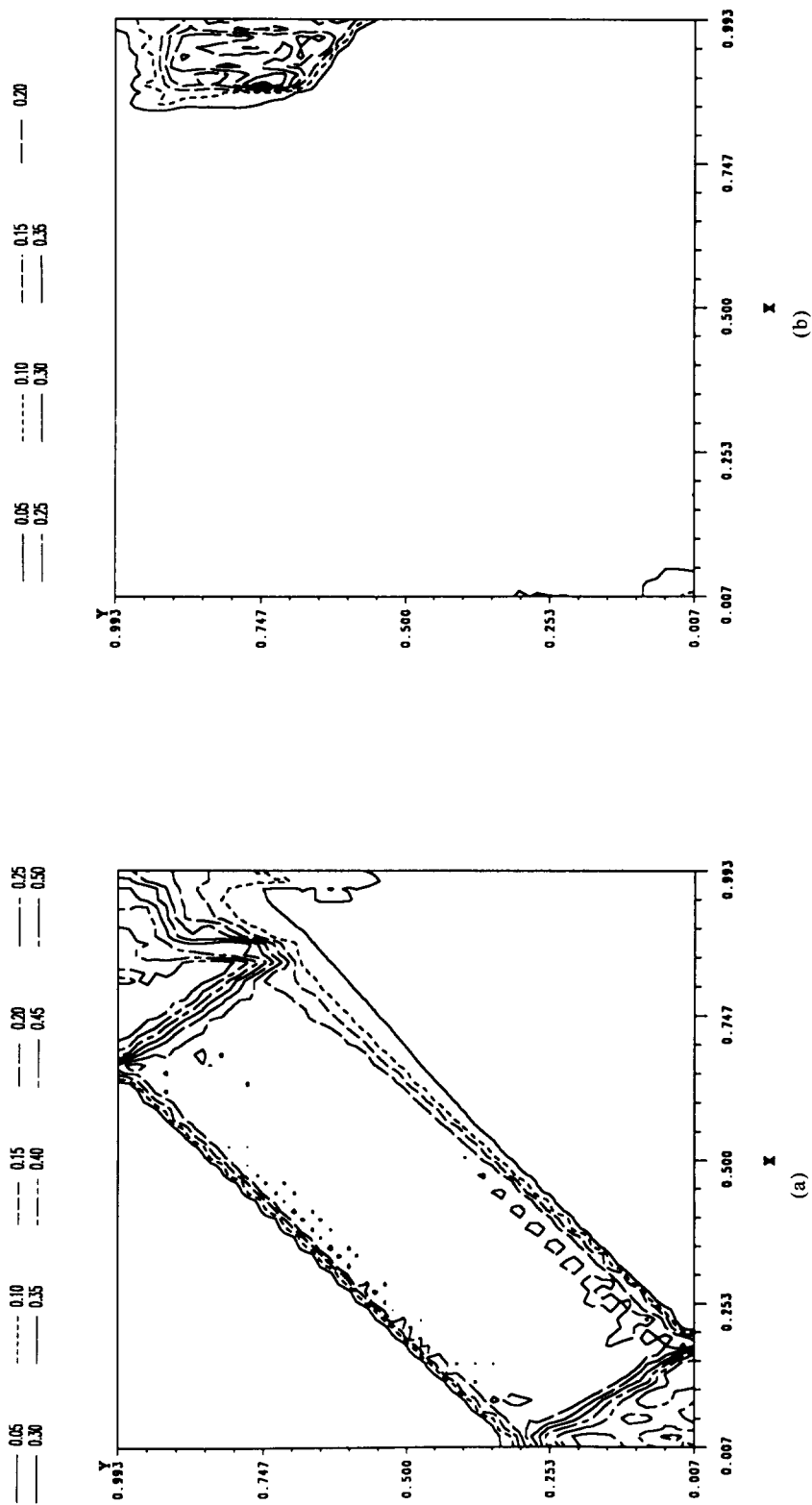


Fig. 14. Contours of the accumulated plastic slip strain in different slip systems at an average strain of 0.10755. (a) Slip systems (111)[110] and (111)[011], (b) Slip systems (111)[110] and (111)[011]. (Figure continues)

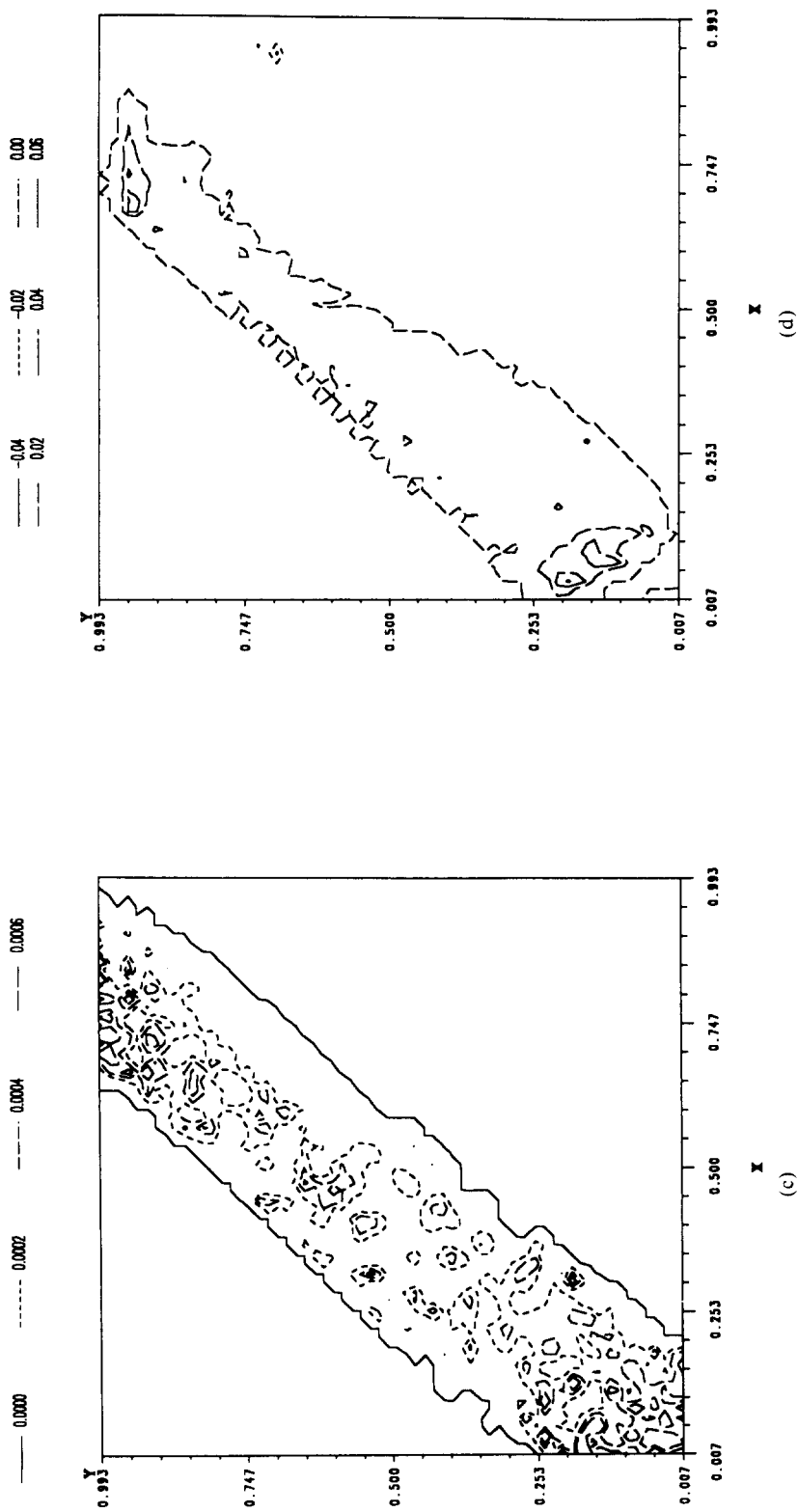


Fig. 14. (c) Slip systems $(111)[011]$ and $(111)[101]$, (d) Slip systems $(111)[101]$ and $(111)[011]$. (Figure continues)

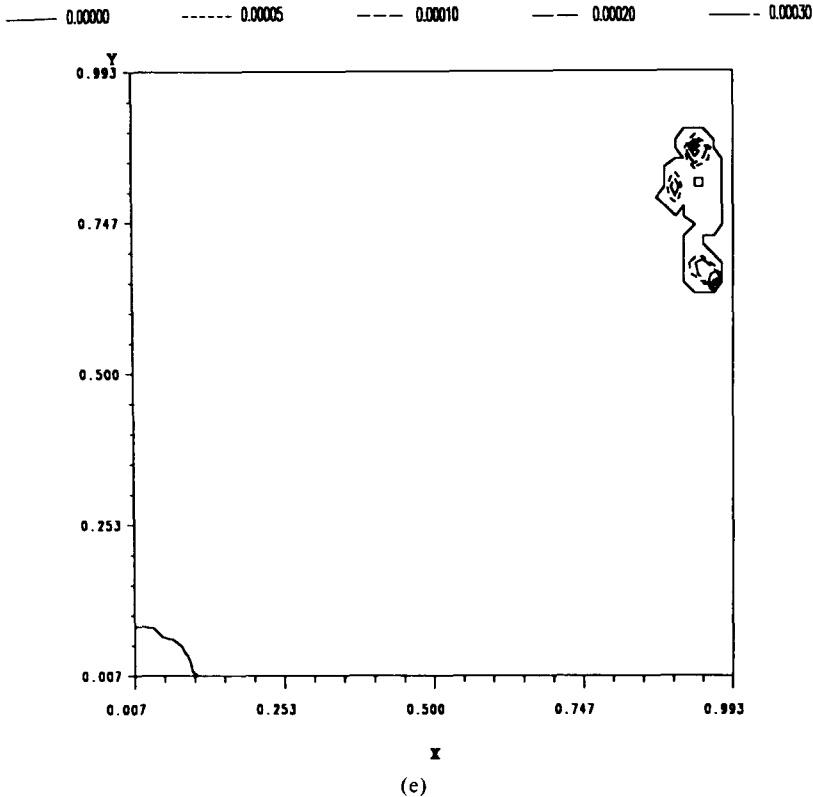


Fig. 14. (e) Slip systems $(11\bar{1})[1\bar{1}0]$ and $(\bar{1}11)[0\bar{1}1]$.

IV. CONCLUSIONS

We have studied the problem of the initiation and growth of dynamic shear bands in an fcc single crystal deformed in simple compression along the direction $[010]$ of the crystal at a nominal strain-rate of 1000 sec^{-1} . The coupled nonlinear partial differential equations governing the dynamic thermomechanical plane-strain deformations of the single crystal are solved numerically. Two different cases, namely, when the plane of deformation is parallel to the plane (001) or $(10\bar{1})$ of the single crystal, are analyzed. In each case, the deformations are assumed to be symmetric about the horizontal and vertical centroidal axes, and all 12 slip systems are taken to be active. However, only those slip systems for which the resolved shear stress equals or exceeds the critical shear stress contribute to the plastic deformation. The effects of isotropic hardening, kinematic hardening, and thermal softening are incorporated in the expression for the critical shear stress. The deformations of the material in the first quadrant are examined closely.

It is found that when the plane of deformation is parallel to the plane (001) of the single crystal, a single shear band originates from the center of the cross-section and propagates along a line making an angle of 45° with the horizontal. The band is reflected back from the top loading surface, the angle of reflection being nearly equal to the angle

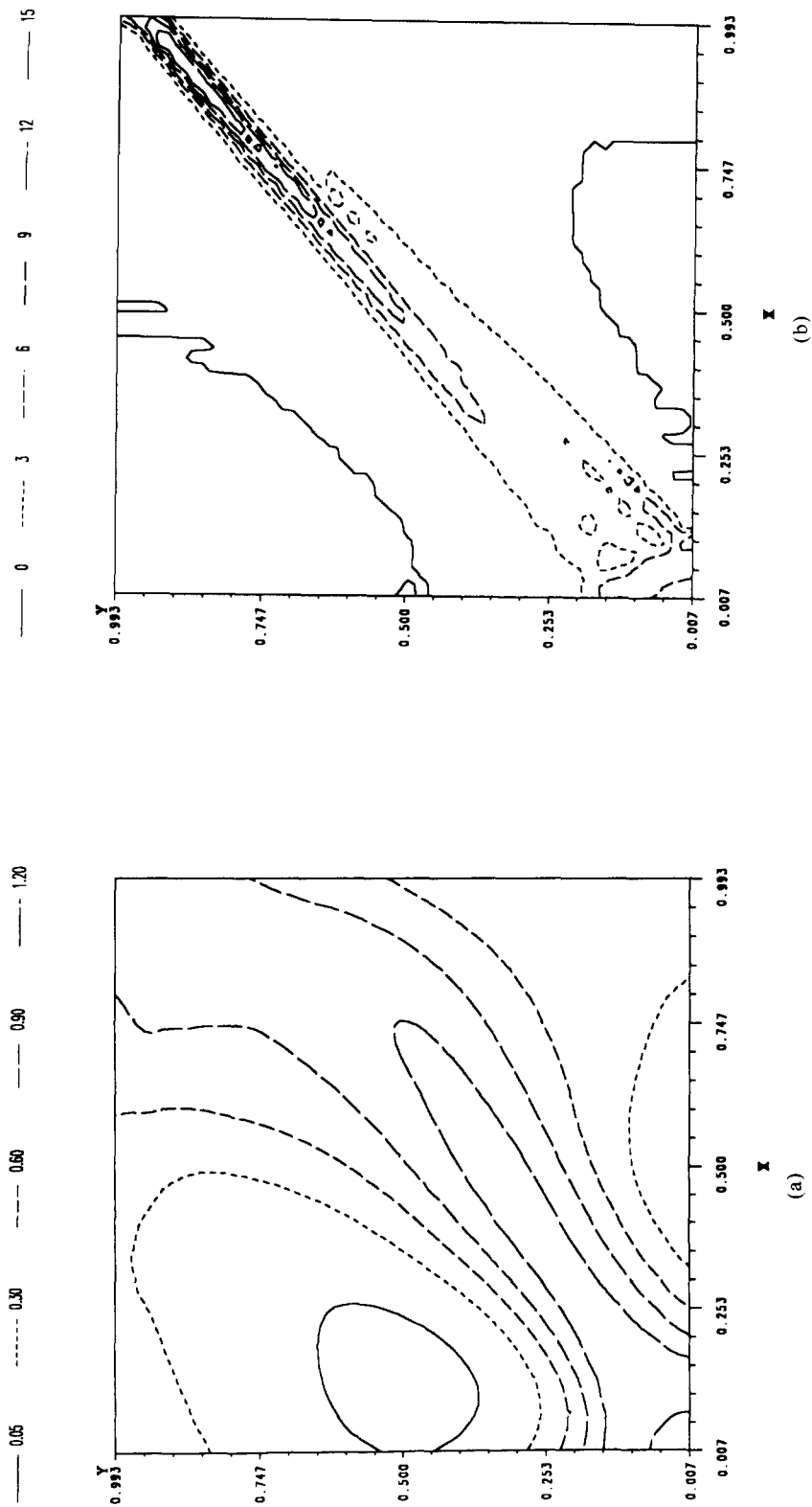


Fig. 15. Contours of the slip strain-rate of slip systems $(111)[110]$ and $(111)[011]$ (a, b, c) and that of slip systems $(111)[110]$ and $(111)[011]$ (d, e, f) at three different values, 0.00255, 0.02755, and 0.10755, of the nominal strain. (Figure continues)

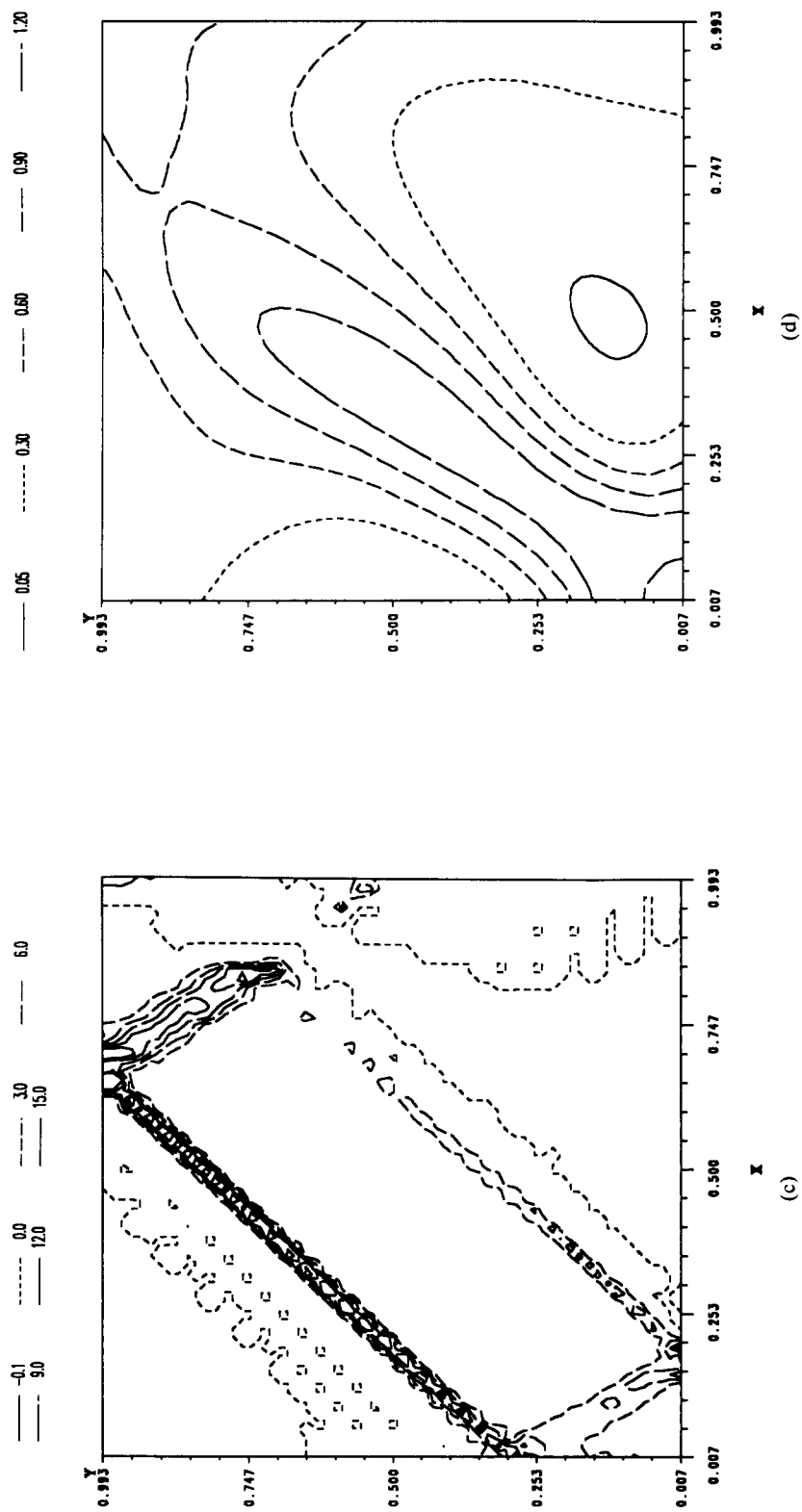


Fig. 15. (c, d). (Figure continues)

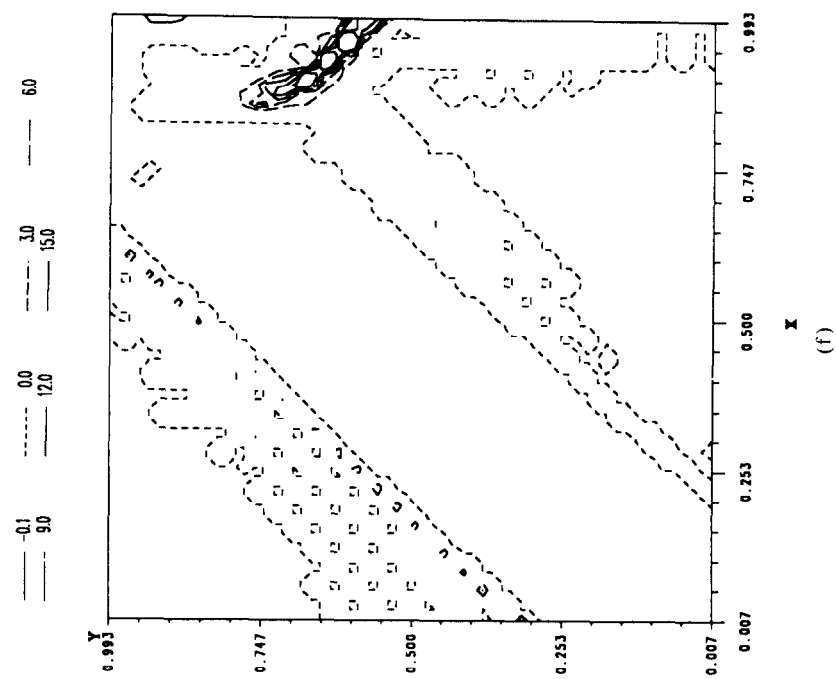
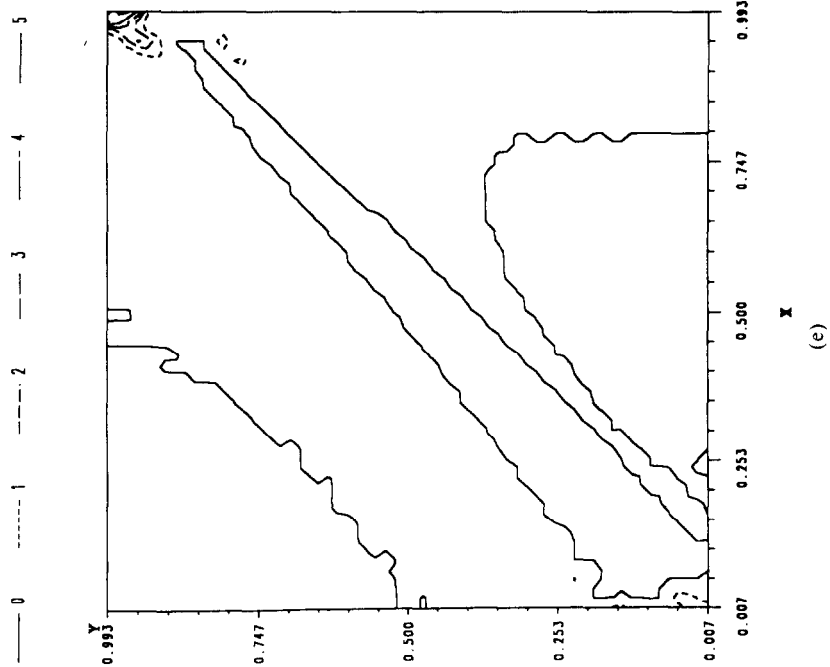


Fig. 15. (e, f)

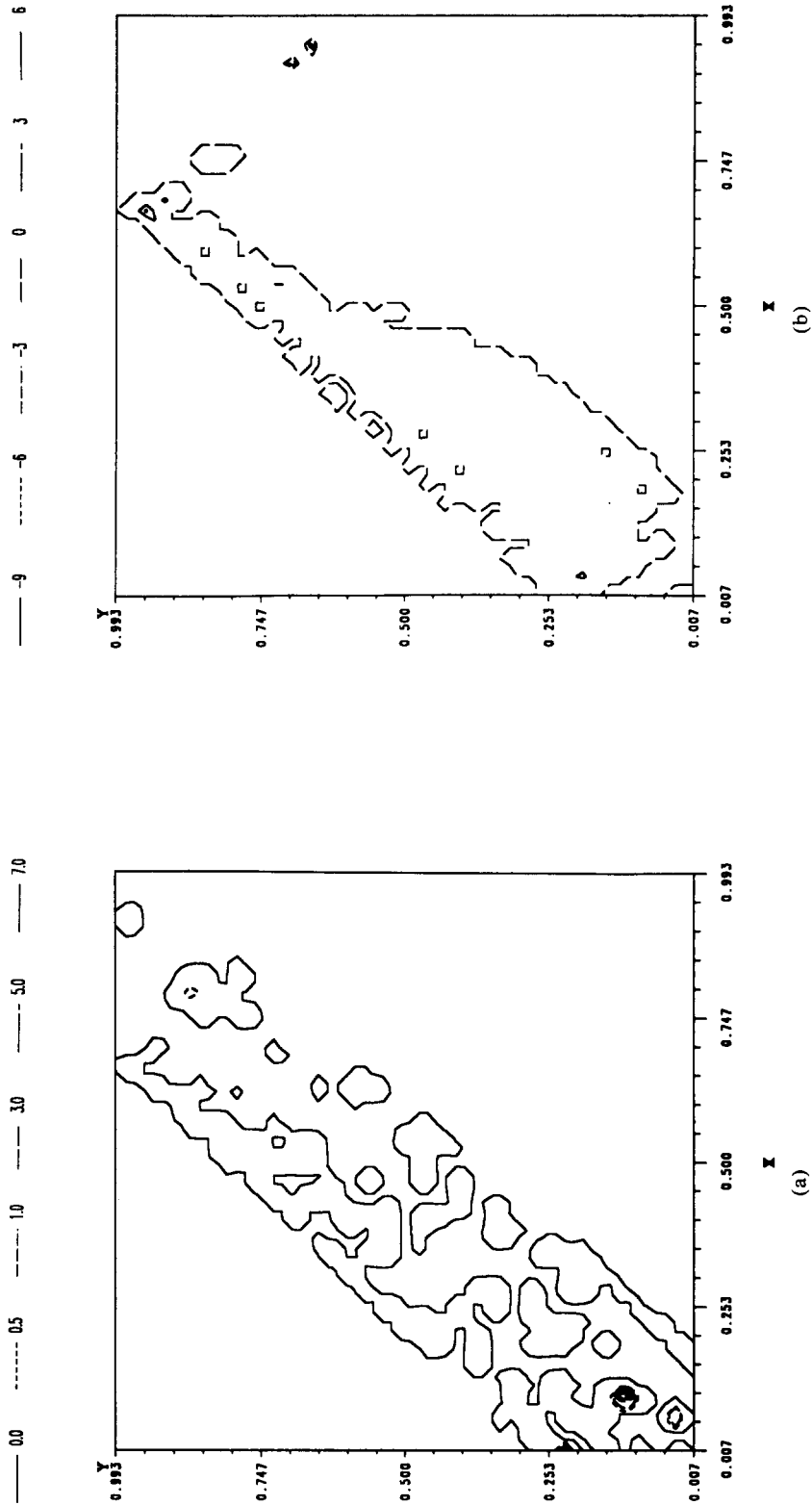


Fig. 16. Contours of the slip strain-rates of different slip systems at an average strain of 0.10755. (a) Slip systems $(111)[011]$ and $(111)[110]$, (b) Slip systems $(111)[101]$ and $(111)[101]$. (Figure continues)

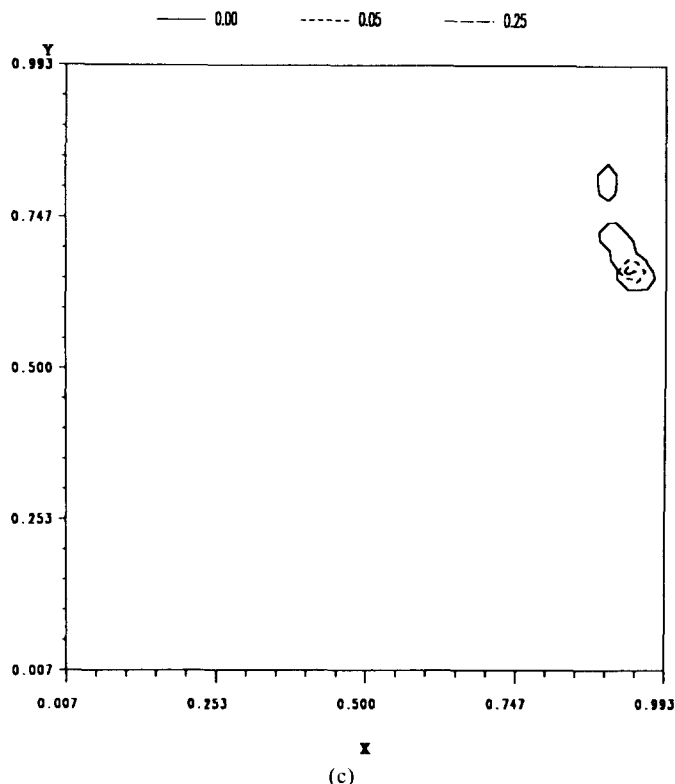


Fig. 16. (c) Slip systems $(11\bar{1})[1\bar{1}0]$ and $(\bar{1}11)[0\bar{1}1]$.

of incidence. The slip strains on the slip systems $(111)[1\bar{1}0]$, $(11\bar{1})[1\bar{1}0]$, $(1\bar{1}\bar{1})[110]$, and $(1\bar{1}1)[110]$ are very high, and these four slip systems are the primary slip systems. The slip systems $(111)[0\bar{1}1]$, $(11\bar{1})[0\bar{1}\bar{1}]$, $(1\bar{1}\bar{1})[101]$, and $(1\bar{1}1)[10\bar{1}]$ in the central band, and slip systems $(111)[10\bar{1}]$, $(11\bar{1})[101]$, $(\bar{1}11)[0\bar{1}1]$, and $(1\bar{1}1)[011]$ in the reflected band are the conjugate slip systems. At a nominal strain of 0.10755, the average angle of rotation of the crystal lattice within the central band is 14.5° counterclockwise, its maximum value is 18.54° counterclockwise, the average angle of rotation in the reflected band is 14.3° clockwise, and its maximum value is 20.29° clockwise.

When the plane of deformation is parallel to the plane $(10\bar{1})$ of the single crystal, the shear band originating from the center of the cross-section propagates along the line making an angle of 39.5° with the horizontal, and eventually splits into two bands. The intensity of slip-rate in the upper band is higher than that in the lower band. The upper band is reflected from the top surface, and this reflected band stops the lower band from reaching the top surface of the cross-section. Two slip systems, $(111)[10\bar{1}]$ and $(1\bar{1}1)[10\bar{1}]$, remain inactive throughout the entire loading history. Slip systems $(111)[1\bar{1}0]$ and $(111)[0\bar{1}1]$ in both the central and the reflected band, and slip systems $(1\bar{1}1)[110]$ and $(1\bar{1}1)[011]$ in the reflected band were found to be more active than other slip systems. The average value of the angle of rotation of the crystal lattice, at a nominal strain of 0.10755, equalled 22.9° counterclockwise in the central band, and 17.2° clockwise in the reflected band.

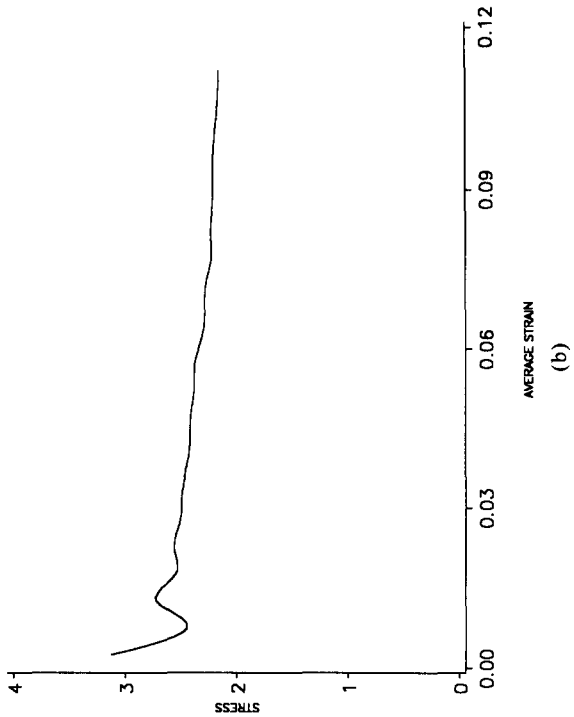
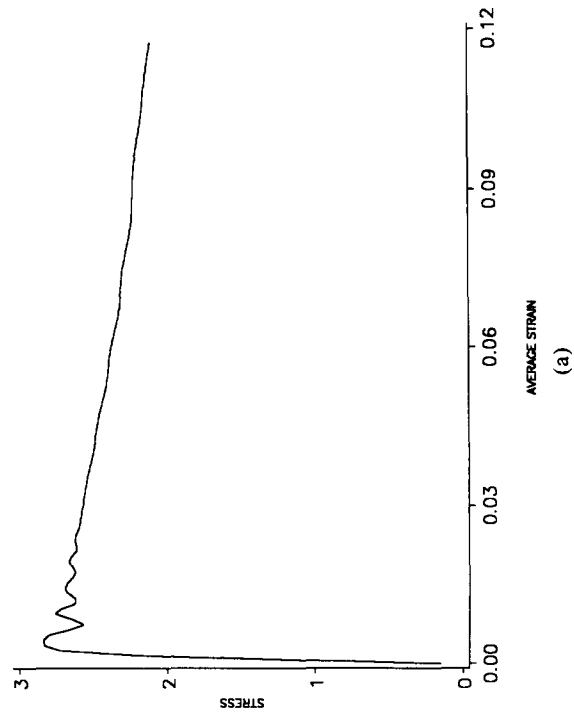


Fig. 17. Average axial stress vs. the average axial strain for the two cases studied. (a) Plane of deformation is parallel to the plane (001) of the single crystal, (b) Plane of deformation is parallel to the plane (101) of the single crystal.

Acknowledgements—This work was supported by the US Army Research Office grant DAAL03-91-G-0084 and the US NSF grant MSS9121279 to the University of Missouri–Rolla. Some of the computations were performed on the NSF sponsored supercomputer center in Ithaca, NY.

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(Received 4 June 1992; in final revised form 5 November 1992)