NUMERICAL ANALYSIS OF THE ONSET OF SHEAR BAND AND THE POST SHEAR BANDING DEFORMATION OF FCC CRYSTALS

J. Nitta*, S. Kanno†, K. Ito* and T. Sagawa†

*Graduate School of Information Sciences, Tohoku University, Aoba-ku Sendai 980-8579, Japan
†Department of Intelligent System Engineering, Ichinoseki National College of Technology, Hagisho Ichinoseki 021-8511, Japan

Key words: Ductile Fracture, Finite Element Polycrystal Method, Crystalline Plasticity, Localized Shear Banding, Post-Bifurcation

Abstract. We performed numerical analyses, based on crystalline plasticity, of the formation and development of localized shear bands in ductile single crystals in order to establish a fundamental basis for predicting the forming limit of sheet metals. We predict the critical condition and direction of the development of shear bands using bifurcation theory. The elasto-plastic constitutive equation and shear band bifurcation conditions proposed by Asaro are extended to three dimensions. For three-dimensional face centered cubic single crystals which possess 12 slip systems, we perform eigenvalue analyses of the acoustic tensor obtained using an equilibrium equation in which a shear band mode is assumed. Using rate-independent crystalline-plasticity constitutive equations, the number of slip systems involved in the formation of the shear band and the method of selection of their combinations greatly affect the results of bifurcation analysis. In this study, we determine five slip systems using our new standards. In order to assure the positive definite constitutive tensors, we adopt a modified independent hardening rule. For the post-bifurcation analysis, we introduce a hypothetical 13th slip system into elements that satisfy the bifurcation conditions. Results of numerical analyses applied for plane strain compression and plane strain tension demonstrate that an envelope line connecting shearing directions of elements penetrates the sheet metal in the thickness direction. We define the moment the metal is penetrated as the stage of fracture of the metal.
1 INTRODUCTION

Localized necking, which appears prior to fracture, in the forming of sheet metals is important since its development is considered to indicate the forming limit. Much research on plastic instability behavior has previously been reported by, for example, Hill [1], Stören and Rice [2] and Hill and Hutchinson [3]. They discussed shear bands on a plane stress field based on the bifurcation theory. Ito et al. [4] analyzed problems which predict the rupture-limit strain of sheet metals using the three-dimensional localized bifurcation theory. These studies were performed from the viewpoint of macrocontinuum mechanics. Meanwhile, since shear band phenomena develop in a microscale localized field smaller than crystal grain sizes, these phenomena are considered to be affected by the crystal structure of metal materials. Accordingly, there is a limitation in the approach using conventional continuum mechanics, thus analyses using the crystalline plasticity theory are required. Asaro [5] and Pierce et al. [6] used idealized symmetry double-slip models which were based on the bifurcation theory emphasizing crystalline plasticity, and obtained an analytical solution for bifurcation of a shear band of uniaxial tension in ductile single crystals. These planar double-slip models are extremely simplified and they are not applicable to general deformation. Therefore, we consider that the discussion of the characteristics of shear bands obtained by these double-slip models were only qualitative, and that it is difficult to apply these models to the prediction of the actual forming limit of metals. Recently, Anand et al. [7] clarified the effects of the crystallographic structure of fcc materials with 12 slip systems during a shear band formation process in plane strain compression, by means of numerical simulation and experimental observations. In their research, a numerical model regarding the formation and development of shear bands was not introduced.

In this research, we use the finite element polycrystal model proposed by Takahashi et al. [8] and extend the method by Asaro et al. [5] to a three-dimensional one; then we perform numerical analyses of localized shear bands based on the mechanism of crystalline plasticity, with consideration given to the crystal structures of actual materials. Subsequently, we assume the shear band to be a hypothetical nonhardening 13th slip system for each grain of fcc crystal that satisfy the bifurcation conditions, and consider that the shear band contributes to the deformation of a material. We then perform post-bifurcation analyses. Based on the results, we discuss the load-deformation diagram, the formation of shear bands and the relationship between its development and rupture of sheet metals.

2 BIFURCATION ANALYSIS

We assumed that the slip direction vector $s^{(\alpha)}$ and a slip-plane normal vector $m^{(\alpha)}$ are given in an active slip system $\alpha$ in the deformation of single crystals, where superscript within ( ) means the number of the slip system. The Schmid tensor $p^{(\alpha)}$ which defines the strain rate and $\omega^{(\alpha)}$ which defines the plastic spin of a crystal coordinate system are
given by
\[
\begin{align*}
\mathbf{p}^{(\alpha)} &= \frac{1}{2}(\mathbf{s}^{(\alpha)}\mathbf{m}^{(\alpha)} + \mathbf{m}^{(\alpha)}\mathbf{s}^{(\alpha)}) \\
\omega^{(\alpha)} &= \frac{1}{2}(\mathbf{s}^{(\alpha)}\mathbf{m}^{(\alpha)} - \mathbf{m}^{(\alpha)}\mathbf{s}^{(\alpha)})
\end{align*}
\]  
(1)

Using Eq.(1), the plastic shear strain rate of each slip system \(\dot{\gamma}^{(\beta)}\) relative to the strain rate tensor of crystal \(\mathbf{D}\) is given by
\[
\dot{\gamma}^{(\beta)} = \sum_\alpha \left\{ h_{\alpha\beta} + \mathbf{P}^{(\alpha)} : \mathbf{C} : \mathbf{P}^{(\beta)} \right\}^{-1} \mathbf{P}^{(\alpha)} : \mathbf{C} : \mathbf{D}
\]  
(2)

\(C\) : elastic coefficient matrix
\(h_{\alpha\beta}\) : hardening matrix

Considering lattice rotation, Schmid tensor is rewritten as Eq.(3) and the relationship between \(\mathbf{D}\) and Jaumann rate of the Cauchy stress \(\overline{\mathbf{\sigma}}\) can be given by Eq.(4).
\[
\begin{align*}
\hat{\mathbf{p}}^{(\alpha)} &= \mathbf{p}^{(\alpha)} + C^{-1} \cdot \left( \omega^{(\alpha)} \cdot \mathbf{\sigma} - \mathbf{\sigma} \cdot \omega^{(\alpha)} \right) \\
\overline{\mathbf{\sigma}} &= C : \left\{ \mathbf{D} - \sum_\alpha \hat{\mathbf{p}}^{(\alpha)} \dot{\gamma}^{(\alpha)} \right\}
\end{align*}
\]  
(3)  
(4)

In the deformation of ductile sheet metals, we consider the deformation upon the formation of a shear band in the macroscopic coordinate system \(x, y\) and \(z\), shown in Figure 1, as follows: with respect to the deformation in the \(x\)-axis direction, discontinuity in the
velocity gradient develops at the boundary plane where \( n \) is the normal, and the resulting discontinuity in the velocity is given by Eq.(5) below. Here, \( f(n \cdot x) \) is an arbitrary function whose second-order differential is not zero.

\[ v = f(n \cdot x)g \]  

(5)

With this equation, there is no difference in the velocity gradients in a direction parallel to the shearing plane between inside and outside of the boundary where the shear band forms, however, velocity gradient differences exist in the \( n \)-direction. \( g \) is a unit vector in a direction representing the discontinuity of the velocity. When the discontinuity shown by Eq.(5) occurs, Eq.(6) can be obtained from an equilibrium equation of nominal stress. \( Q \) is a second-order tensor called acoustic tensor, which is a function only of \( n \), when a stress state is specified.

\[ Q(n, \sigma) \cdot g = 0 \]  

(6)

Therefore, when Eq.(6) has a nonzero solution with respect to \( g \), a shear band may form first, indicating the bifurcation; Eq.(7) gives the condition required for the formation of shear band.

\[ |Q(n, \sigma)| = 0 \]  

(7)

Eq.(7) is solved by eigenvalue analysis. First we calculate stress using the given strain, the minimum eigenvalue for \( Q \) with respect to all plane normal directions \( n \) for each element, and then \( n \) and \( g \) are obtained when the minimum eigenvalue of element becomes 0. The resultant \( n \) and \( g \) are the normal to the plane and the slip direction of the shear band, respectively, in that element.

In the bifurcation analysis based on the rate-independent crystalline plasticity, results significantly depend on the combination and the number of slip systems involved in the formation of shear band. Nonetheless, there are no appropriate guidelines for these problems. These are extremely important and difficult problems, and there are other points to be considered in addition. In this study, we determined the following standards and conditions for analyses, based on the results of various examinations.

1) We set the number of slip systems to five, considering the degrees of freedom in incompressible deformation. Then we selected consecutive slip systems starting from the slip system in which larger resolved shear stress is acting. Another possible method is to calculate the plastic work for all combinations of 5 slip systems from the total of 12 slip systems, and to select the combination which has the minimum plastic work value. However, this method is not feasible due to the restriction of computation time. Since a slip system which has large resolved shear stress has a greater effect on the deformation, it is reasonable to consider that this slip system also significantly affects the formation of shear bands.

2) To examine linear independence of the combination of selected slip systems, we evaluate the Gramian \( G_{ij} \) composed of Schmid tensors of 5 slip systems. When
a combination does not satisfy Eq.(8), we replace a slip system with another slip system until a satisfactory combination is found. Since the Gramian is almost equivalent to the second term inside \{ \} of Eq.(2), satisfaction of Eq.(8) guarantees to be able to calculate inverse matrix regardless of work hardening rate matrix \( h_{\alpha\beta} \).

\[
| G_{ij} | = | p^i : p^j | \neq 0 \tag{8}
\]

c) In the calculation of \( \dot{\gamma}^{(\beta)} \) in Eq.(2), since restrictions corresponding to the amount of resolved shear stress should be applied to each of the 5 slip systems, we use the modified hardening rate matrix shown in Eq.(9). In Asaro’s theory, the magnitude of the resolved shear stress does not affect the formation of shear band. However we constructed the system so that the larger the resolved shear stress, the larger the contribution to \( \dot{\gamma}^{(\beta)} \). This is the basis of the rate-dependent model. The value of \( m \) is the exponent which constrains the amount of slip. When \( m \) is zero, Eq.(9) reduces to the Schmid’s law.

\[
h_{\alpha\beta} = h \delta_{\alpha\beta} \left( \frac{k^{(\beta)}}{\tau^{(\beta)}} \right)^m \tag{9}
\]

\( k^{(\beta)} \) : yield stress
\( \tau^{(\beta)} \) : resolved shear stress
\( h \) : hardening rate
\( m \) : constraint exponent

In the case of latent hardening model, the positive definite characteristic of constitutive equation (4) is not always satisfied. So we adopt independent hardening model by Eq.(9).

3 POST-BIFURCATION ANALYSIS

Most studies have focused on the analyses of shear band bifurcation and the effects of micro structure on shear banding condition. However, elements in which shear bands form are expected to weaken due to the changes in the structures and stress conditions; and thus, analyses after the formation of shear bands, i.e., post-bifurcation analyses, are required. In this study, the normal line of the shear band plane of each element \( n \) and the direction of slip \( g \) are obtained using the eigenvalue analysis, and this shear band is assumed to be the new 13th hypothetical slip system of the element. Schmid tensor \( p^{(13)} \) which defines the strain rate of the 13th slip system, and \( \omega^{(13)} \) which defines the plastic spin, are expressed by

\[
\begin{align*}
p^{(13)} &= \frac{1}{2} \left( g^{(13)} n^{(13)} + n^{(13)} g^{(13)} \right) \\
\omega^{(13)} &= \frac{1}{2} \left( g^{(13)} n^{(13)} - n^{(13)} g^{(13)} \right)
\end{align*} \tag{10}
\]
The hardening rule of the slip system is assumed to be nonhardening rule with initial yield stress which is the resolved shear stress when the bifurcation condition is satisfied, as expressed by Eq.(11).

\[ k^{(13)} = \tau^{(13)}_{\text{crit}} = [p^{(13)} : \sigma]_{\text{crit}} \]  

\[ \tau^{(13)}_{\text{crit}} : \text{resolved shear stress at shear banding} \]

Post-bifurcation deformation analyses were performed using the finite element model, which was modified so that this new slip system also contributes to plastic deformation and plastic rotation, similar to the other slip systems.

4 RESULTS

Results of plane strain compression and plane strain tension of fcc single crystals are shown. The material properties used in calculation are listed in Table 1.

<table>
<thead>
<tr>
<th>Elastic properties</th>
<th>$E = 70 \text{ GPa}, \quad \nu = 0.3$</th>
</tr>
</thead>
</table>
| Hardening properties | deformation analysis  
\[ k^{(\beta)} = k_0 + h \Gamma, \quad \Gamma = \int \sum |\dot{\gamma}^{(\alpha)}| \, dt \]  
\[ k_0 = 5 \text{MPa} \]  
\[ h = 100 \text{MPa} \]  

shear band analysis  
\[ h_{\alpha\beta} = h \delta_{\alpha\beta} (k^{(\beta)}/|\tau^{(\beta)}|)^m \]  
\[ k^{(\beta)} : \text{yield stress} \]  
\[ \tau^{(\beta)} : \text{resolved shear stress} \] |

Table 1: Material properties used for calculation

4.1 Plane strain compression

The mesh size of the finite element model is (16 16 1). Figure 3 shows the initial shape; Figure 4 and Figure 6 show the shapes after deformation. This model represents a part of the sheet metal which is subjected to plane strain compression in the thickness direction of the metal. The relationship between the macroscopic coordinate system ($x, y, z$) and the crystalline coordinate system ($x', y', z'$) is represented using the Euler angles.
Figure 2: Euler angle ($\theta$, $\phi$, $\psi$)

Figure 3: Undeformed finite element meshes of single crystals under plane strain compression.
Figure 4: Deformed finite element meshes of single crystals under plane strain compression. ($|\varepsilon| = 0.14$)

Figure 5: Pole figure of shear band direction of the elements forming the envelope under plane strain compression.
shown in Figure 2; the initial directions, i.e. $\theta$, $\phi$ and $\psi$, of the single crystals used for the calculation are $20^\circ$, $-10^\circ$ and $0^\circ$, respectively. Where $x$-axis is compressive direction and $z$-axis is constraint one. The elements painted in Figure 4 are those satisfying the bifurcation conditions at a mean compressive strain below 0.14; these elements account for approximately 40% of all elements. When the mean compressive strain is 0.04, bifurcation element begins to appear and advance almost symmetrically from the periphery to the center of the material, resulting in the linear connection of bifurcation elements. The $g$ vectors of each bifurcation element align almost in one direction, and the envelope line connecting these vectors penetrates the metal layer. The envelope line is almost straight, and the angle formed between it and the $x$-axis is $56^\circ$. Pole figure of shear band direction of the elements located on the envelope line is shown as Figure 5. When the envelope line penetrates the metal layer, we assume that a shear band penetrates the sheet metal and a fracture occurs. The shape in Figure 6 shows the state in which deformation further
advances with a mean compressive strain of 0.33; the shape deformation of elements positioned on the penetration line appears to be large, and fracture is expected at the penetration line. Figure 7 shows the relationship between mean compressive stress and mean compressive strain. In Figure 7, solid line and dash line are in the case of with and without the 13th slip system respectively. Point A is the starting point of the bifurcation of the elements (mean strain : 0.04), and point B is the penetration point of the envelope line (mean strain : 0.14). The mean stress with the 13th slip system is less than that without the 13th slip system, indicating the softening of the material due to the formation of the shear band. After the occurrence of shear band penetration, significant relative softening of the material can be seen. Bifurcation elements not located on the penetration line are not related to fracture, even when those elements appear at an early stage. We were able to obtain these results using the post-bifurcation analysis.

4.2 Plane strain tension

Figure 8 shows the finite element model of a part cut out from the sheet metal under plane strain tension. The mesh size is set as (30 10 1), and the center is reduced by a maximum of 8% so that the edge lines have the shape of a sine wave. Here $x$-axis and $z$-axis are the tensile direction and the constraint one. The initial Euler angles $\theta$, $\phi$ and $\psi$, are $30^\circ$, $-15^\circ$ and $0^\circ$, respectively. The elements painted in Figure 9 indicate those satisfying the bifurcation conditions at a mean tensile strain below 0.45, and at this strain some of these elements are connected in the thickness direction of the sheet metal. The number of such elements accounts for approximately 70% of all elements. The bifurcation elements begin to appear at the mean tensile strain of 0.06, and advance almost symmetrically from both longitudinal edges as well as from the upper and bottom surfaces to the center of the metal. And they are connected in the thickness direction of the metal at the mean strain of 0.45. Similar to the case of plane strain compression, $g$ vectors of bifurcation elements align almost in one direction, and the envelope line connecting these vectors is almost straight. The envelope line penetrates the metal layer, forming an angle of 32° with the $x$-axis. This moment is defined as the moment of fracture. Pole figure of shear band direction of the elements forming the envelope is shown in Figure 10. Figure 11 shows the case with the mean tensile strain of 0.86, in which the development of fracture is unrecognizable from the shape change. Figure 12 shows the relationship between mean tensile stress and mean tensile strain. When the 13th slip system is introduced, the mean stress begins to decrease at point A (mean strain : 0.06), and significant relative softening can be seen after the point B (mean strain : 0.45), where the envelope line penetrates the metal layer. And the bifurcation elements from an early stage are not necessarily related to fracture.
Figure 8: Undeformed finite element meshes of single crystals under plane strain tension.

Figure 9: Deformed finite element meshes of single crystals under plane strain tension. ($|\varepsilon| = 0.45$)

Figure 10: Pole figure of shear band direction of the elements forming the envelope under plane strain tension.
Figure 11: Deformed finite element meshes of single crystals under plane strain tension. (|\varepsilon| = 0.86)

Figure 12: Average nominal stress \(\sigma\) vs average tensile strain \(\varepsilon\). Shear band was formed first at A and penetrated at B.
5 CONCLUDING REMARKS

We performed numerical analyses of the bifurcation and the post-bifurcation of localized shear bands due to deformation by plane strain compression and plane strain tension on fcc single crystals, and obtained the following results.

a) We proposed some new standards and conditions for the bifurcation analyses based on the rate-independent crystalline plasticity.

b) Localized shear bands advance almost symmetrically from the periphery to the center of the material.

c) Slip direction vectors of a shear band of each bifurcated element align almost in one direction for both cases of compression and tension. The envelope line connecting these vectors is straight and penetrates the metal layer. The penetration line and the compressive, tensile direction form angles of 56° and 32° respectively.

d) There is a fairly large difference in the value of strain between that when a shear band first forms in an element and that when the envelope line of shear bands penetrates the metal layer. The moment of penetration is defined as the moment of the development of fracture.

e) The elements which form a shear band at an early stage do not necessarily relate to fracture.

f) Numerical results by introducing a shear band as the 13th hypothetical slip system, show lower mean stress, that is relative softening of the material, compared to the case without the 13th slip system. Significant effects of softening can be observed after the penetration of the shear band into the metal layer.

References


