Finite Element Model of Arbitrary Inclined Edge Dislocations*

Kazuaki SASAKI**, Md Sham Miri Abd RAHMAN***
and Michiya KISHIDA****

In considering mechanical behavior of crystals, it is very important to know the elastic incompatible stresses near the dislocation, which plays an important role in elasto-plastic deformation. The authors proposed a finite element model of an edge dislocation, based on the mathematical model of dislocation. In this paper, a finite element model of an arbitrary inclined edge dislocation is proposed by the use of a discrepancy of displacement, and the stresses around an edge dislocation in an infinite region are obtained and compared with exact solutions. In this analysis, opening mode discrepancy of displacement and shear mode discrepancy of displacement are located along the same line, and the corresponding nodal points are connected with each other. Also, the problem with two edge dislocations is treated. The results coincide with exact ones.

Key Words: Elasticity, FEM, Numerical Analysis, Edge Dislocation, Inclined Dislocation, Discrepancy of Displacement, Superposition

1. Introduction

A concept of dislocation has been introduced by Volterra⁽¹⁾ for the first time, and used to explain a slip in crystal by many researchers so far. It is no exaggeration to say that a dislocation is one of important factors, which decides dynamic characteristics of crystal when thinking of a slip in crystal. Generally, an analytical method is used to obtain mechanical behavior around dislocation, and so the analysis of complicated shapes and under complicated boundary conditions is difficult. The authors proposed the finite element dislocation model⁽²⁾ to obtain stresses and displacements around an edge dislocation, based on a

mathematical model of dislocation⁽¹⁾. In that paper, stress field around an edge dislocation was obtained in a circular region and in an infinite region, and the availability of this dislocation model was shown by the comparison with the analytical result. Also, we examined an elastic incompatible stress near a triple subgrain boundary⁽³⁾ by considering a grain boundary as continuous distribution of dislocation.

By the way, in actual metallurgical material, grain boundaries and inclusions often exist near the dislocation, and the stress analysis around such dislocation is important. The problem of this kind can be analyzed also by the finite element dislocation model above-mentioned, but generally, we must think that plural dislocations exist with arbitrary angles to boundaries. When we limit our discussion to a mechanical behavior in linear elasticity, the problem can be solved by decomposing Burger's vector and by superposing stress fields of each problem. However, for superposition of stress fields, it is necessary for nodal points after deformation to coincide with each other, and so, element subdivision needs great labor. In this paper, we propose a finite element model to analyze an arbitrary inclined dislocation problem by introducing shear- and opening-mode discrepancies of

* Received 3rd October, 2001. Japanese original: Trans. Jpn. Soc. Mech. Eng., Vol. 66, No. 651, A (2000), pp. 1977-1983 (Received 27th July, 1999)

** Division of Mechanical Science, Graduate School of Engineering, Hokkaido University, N-13 W-8, Kita-ku, Sapporo 060-8628, Japan. E-mail: kazki@eng.hokudai.ac.jp

*** Department of Mechanical Engineering, Faculty of Engineering, Hokkaido University (Present Address: ALPS ELECTRIC Co., Ltd)

**** 2-4-10-30 Tonden, Kita-ku, Sapporo 002-0852, Japan

displacement, and show a possibility to obtain stress field. As an example, an arbitrary inclined edge dislocation in an infinite region is treated and a usefulness of this method is shown by comparison with exact results.

Moreover, the modeling of plural dislocation is examined by introducing plural discrepancies of displacement on the same discrepancy line. Stress distribution around arbitrary inclined two edge dislocations in an infinite region is obtained and compared with exact results, i.e. superposition of the result of one edge dislocation problem.

2. Finite Element Model

In this paper, we treat the model of one or two edge dislocations with arbitrary inclination. An edge dislocation can be represented by mathematical model⁽¹⁾ where the discrepancy of displacement, given as the equal size to Burgers vector, is joined with one another as shown in Fig. 1. Authors have proposed the finite element model of dislocation based on this mathematical model and have shown that the mechanical field around dislocation can be obtained accurately⁽²⁾. Hereafter, we call the discrepancies of dislocation, corresponding to Figs. 1(a) and (b), as opening- and shear-mode discrepancies of displacement, respectively.

In this paper, we propose the finite element model of arbitrary inclined edge dislocation where the components of discrepancy of displacement in x - y coordinates system is given by decomposed components of the Burgers vector, respectively. This model is based on a fact that we can apply the principle of superposition to analyze the stress and displacement in linear elasticity. The concept of this model is shown in Fig. 2. The discrepancy of displacement b_y in y -direction can be represented not only by shear-mode discrepancy of displacement in Fig. 2 but also by opening-mode one given on x -axis⁽⁴⁾. From this

Fig. 1 Mathematical model of edge dislocation, (a) Opening-mode discrepancy of displacement, (b) Shear-mode discrepancy of displacement

concept, it is possible to analyze the arbitrary inclined edge dislocation by superposing opening-mode discrepancies in x - and y -directions on different discrepancy lines. The analysis of this model makes an element subdivision complicated; so, we analyze the problem by the model in which opening- and shear-mode discrepancies of displacement are given on the same line. This method has an advantage that element subdivision becomes easier.

The example of the finite element model based on this concept and the detail near the tip of discrepancy are shown in Figs. 3 and 4(a), respectively. Here, the X - Y coordinate system inclined at angle θ in counterclockwise direction to x - y coordinate system is used, that is, the direction of the Burger's vector agrees with X -direction. The rectangular region, width W and length L , is cut along negative y -axis, and the discrepancies of displacement corresponding to b_x and b_y is given on the same discrepancy line. The rectangular region is divided into triangle elements. We divide a region near dislocation ($-50 \leq x/b \leq 50$, $-50 \leq y/b \leq 50$) into regular triangle elements with height b as in Fig. 4(a), expand an element dimension with a distance from dislocation as in Fig. 3 and suppose the rectangular region with $W/b \doteq L/b \doteq 1000$ as approximate infinite region. The tip of a discrepancy is wedge-shaped, and the amount of discrepancy is increased gradually from a tip not to deform the element excessively. The length of the wedge-shaped tip area is determined as $3-4b$ from the fact that the size of dislocation core, where an elastic stress obtained by mathematical model does

Fig. 2 Concept of inclined edge dislocation

Fig. 3 Finite element model of inclined edge dislocation

Fig. 4 Details in region A near a tip of dislocation, (a) The case of one edge dislocation, (b) The case of two edge dislocations

not represent a real stress, is about $5b$. In actual analytical model, the numbers of nodal points and elements are about 15 000 and 30 000, respectively.

Mechanical behavior around arbitrary inclined edge dislocation can be obtained by joining corresponding nodal points on discrepancy line as in Fig. 5. Here, thin and thick lines represent the elements before and after conjunction, respectively. The condition of joining nodal points is

$$\begin{aligned} u_L - u_R &= b_x, \quad v_L - v_R = b_y \\ P_{xL} + P_{xR} &= 0, \quad P_{yL} + P_{yR} = 0 \end{aligned} \quad (1)$$

Here, u and v are x - and y -components of nodal displacement, P_x and P_y those of nodal force, and suffices L and R indicate the amounts on left and right side of discrepancy of displacement, respectively. This condition is same as a method in which equal unknown nodal forces P_{iL} , P_{iR} ($= -P_{iL}$) ($i = x, y$) with opposite direction one another are given on corresponding nodal points to coincide the position of nodal points after conjunction⁽²⁾. In actual computation, this condition is incorporated into stiffness matrix and the solution is obtained at once without iteration. The concrete method to solve stiffness equations is described below.

Fig. 5 Conjunction of nodal points

1. First, the stiffness equation is reconstructed by considering the conditions for nodal force, i.e. equations of P_{xL} , P_{xR} , P_{yL} , P_{yR} in stiffness equations are substituted to Eqs. (1)_{3,4}.

2. Next, the unknown nodal displacements u_R , v_R in stiffness equation are eliminated by considering the conditions for nodal displacements, Eqs. (1)_{1,2}.

3. After all, the numbers of unknowns and stiffness equations are reduced by twos for every connecting condition of neighboring nodal points, and the nodal displacements are completely decided by solving reconstructed stiffness equation.

3. Numerical Results

The results are compared with exact ones of elastic stress field around an edge dislocation with Burger's vector $\vec{b} = b\vec{i}$ in infinite region^{(5),(6)}.

$$\begin{aligned} \sigma_x &= -\frac{Gb}{2\pi(1-\nu)} \frac{y(3x^2+y^2)}{(x^2+y^2)^2} \\ \sigma_y &= \frac{Gb}{2\pi(1-\nu)} \frac{y(x^2-y^2)}{(x^2+y^2)^2} \\ \tau_{xy} &= \frac{Gb}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2} \end{aligned} \quad (2)$$

Here, G is the modulus of transverse elasticity and ν is Poisson's ratio. By replacing x - y coordinate with X - Y coordinate, X - Y components of elastic stresses around arbitrary inclined edge dislocation are obtained. The results are represented by stress index σ_i/σ_0 , τ_{ij}/σ_0 and nondimensional coordinates x/b , y/b . Here σ_0 is a standard stress represented as,

$$\sigma_0 = \frac{G}{400\pi(1-\nu)} \quad (3)$$

Also, the results are shown by the contour lines of stresses. In finite element analysis, stresses at a centroid of each element are obtained by averaging stresses in element itself and neighboring three elements with weight 3:1.

(1) Case of one dislocation

At first, stress fields are obtained for various θ from 0 to $\pi/2$. On account of limited space, the results are shown for $\theta = 0, \pi/8, \pi/4$ in Figs. 6-8. In these

Fig. 6 Stress components in X - Y coordinates system near an inclined edge dislocation, (Numerical results, $\theta=0$)

Fig. 7 Stress components in X - Y coordinates system near an inclined edge dislocation, (Numerical results, $\theta=\pi/8$)

Fig. 8 Stress components in X - Y coordinates system near an inclined edge dislocation, (Numerical results, $\theta=\pi/4$)

Fig. 9 Stress components in X - Y coordinates system near an inclined edge dislocation, (Exact results, $\theta=0$)

Fig. 10 Stress components in x - y coordinates system near two edge dislocations, (Numerical results, $|\vec{b}_2|=|\vec{b}|$, $d/b=28$, $\theta=\pi/2$, $\theta_2=0$)

Fig. 11 Stress components in x - y coordinates system near two edge dislocations, (Exact results, $|\vec{b}_2|=|\vec{b}|$, $d/b=28$, $\theta=\pi/2$, $\theta_2=0$)

Fig. 12 Stress components in x - y coordinates system near two edge dislocations, (Numerical results, $|\vec{b}_2|=|\vec{b}|$, $d/b=28$, $\theta=0$, $\theta_2=\pi/4$)

Fig. 13 Stress components in x - y coordinates system near two edge dislocations, (Exact results, $|\vec{b}_2|=|\vec{b}|$, $d/b=28$, $\theta=0$, $\theta_2=\pi/4$)

results, X - Y components of stresses are shown. The exact stresses, Eq. (2), are shown in Fig. 9. In all cases, it is clear that stresses can be obtained enough accurately except in dislocation core, where exact solution does not represent real stress. These results are easily obtained by turning a coordinate axis of exact solution of $\theta=0$ only by an arbitrary angle. However, it is slightly difficult to obtain exact stress fields around dislocation with arbitrary Burger's vector near free boundary, grain boundary and so on. It is very useful to show that we can obtain any stresses around arbitrary inclined dislocation by finite element method, even though they are numerical results.

(2) Case of two dislocations

Next, we treat two edge dislocations with arbitrary Burger's vectors, and obtain stress field around dislocations. As shown in Fig. 4(b), d is a distance between two dislocations, b_2 and θ_2 are Burger's vector and its inclination of the second dislocation.

The model is a simple superposition of discrepancies of displacement. From this superposition concept, the discrepancy of displacement is given as follows.

$$b_x = |\vec{b}| \cos \theta, \quad b_y = |\vec{b}| \sin \theta \quad (-d \leq y \leq 0)$$

$$b_x = |\vec{b}| \cos \theta + |\vec{b}_2| \cos \theta_2,$$

$$b_y = |\vec{b}| \sin \theta + |\vec{b}_2| \sin \theta_2 \quad (-L/2 \leq y \leq -d)$$

As an example, the problem is treated for (i) $\theta = \pi/2$, $\theta_2 = 0$ and (ii) $\theta = 0$, $\theta_2 = \pi/4$ with $b_2 = b$ and $d/b = 28$. The contour lines of stresses in x - y coordinate system (fixed coordinate system) are shown in Figs. 10 and 12; also, the exact results by superposing exact stresses are shown in Figs. 11 and 13. In any case, it is shown that the stresses around dislocations can be obtained accurately except for neighborhood of dislocation core. From these results, we have confidence that it is possible to analyze stresses around three or more dislocations by the similar model.

4. Conclusions

The finite element model of the arbitrary inclined edge dislocation is proposed based on the mathematical model of dislocation. We propose the model of edge dislocation by superposing opening- and the shear-mode discrepancies of displacement on the same discrepancy line, and make it easy to divide a region into finite elements. As an example, arbitrary inclined edge dislocation in an infinite region is treated, and the applicability of this model with high accuracy is shown by the comparison with exact results. Also, the case of two edge dislocations can be analyzed by similar concept. The possibility to obtain elastic stresses is shown in this paper for arbitrary inclined plural dislocations near free boundary, grain boundary and inclusions by supposing plural discrepancies of displacement on the same line.

Moreover, by superposing the discrepancy in z direction, it is possible to apply this method to mixed dislocation of edge and screw dislocations; this research is under investigation now.

References

- (1) Volterra, V., L'Equilibre des Corps Elastiques-Multiplement Connexes, Ann. Ecole Norm. Super., Vol. 24 (1907), pp. 401-517.
- (2) Kishida, M., Sasaki, K. and Ekida, Y., Dislocation Model in Finite Element Method, Trans. Jpn. Soc. Mech. Eng., (in Japanese), Vol. 63, No. 609, A (1997), pp. 1076-1082.
- (3) Kishida, M., Sasaki, K. and Iwasaki, T., Stress Analysis of a Triple Subgrain Boundary — Examination by Dislocation Model in FEM —, Trans. Jpn. Soc. Mech. Eng., (in Japanese), Vol. 64, No. 620, A (1998), pp. 969-974.
- (4) Sasaki, K., Kishida, M. and Ekida, H., Stress Analysis in Continuous Media with an Edge Dislocation by Finite Element Dislocation Model, Int. J. Num. Method Engng., (in press).
- (5) Taylor, G.I., The Mechanism of Plastic Deformation of Crystals, Proc. Roy. Soc. London, Vol. A145 (1934), pp. 362-405.
- (6) Koehler, J.S., On the Dislocation Theory of Plastic Deformation, Phys. Rev., Vol. 60, No. 1 (1941), pp. 397-410.