ACTA MECHANICA SINICA (English Series), Vol.12, No.3, August 1996 ISSN 0567-7718
The Chinese Society of Theoretical and Applied Mechanics
Chinese Journal of Mechanics Press, Beijing, China
Allerton Press, INC., New York, U.S.A.

A NEW DYNAMIC MODEL FOR STUDY OF DISLOCATION PATTERN FORMATION*

Duan Zhuping (段祝平) Wang Wenbiao (王文标)+ Zheng Qingrong (郑庆荣)+
Huang Guojun (黄国君) Chen Diwen++
(*LNM, Institute of Mechanics, CAS, Beijing* 100080, *China*)
+(*Graduate School, Chinese University of Sciences and Technology, Beijing* 100039, *China*)
++ (Depart. Eng., Clark Atlanta University, Atlanta, GA 30314, USA)

ABSTRACT: Based on the principle given in nonlinear diffusion-reaction dynamics, a new dynamic model for dislocation patterning is proposed by introducing a relaxation time to the relation between dislocation density and dislocation flux. The so-called chemical potential like quantities, which appear in the model can be derived from variation principle for free energy functional of dislocated media, where the free energy density function is expressed in terms of not only the dislocation density itself but also their spatial gradients. The linear stability analysis on the governing equations of a simple dislocation density shows that there exists an intrinsic wave number leading to bifurcation of space structure of dislocation density. At the same time, the numerical results also demonstrate the coexistence and transition between different dislocation patterns.

KEY WORDS: dislocation patterning, diffusion reaction dynamics, variation principle, bifurcation analysis

1 INTRODUCTION

Dislocation pattern[1,2] is a kind of highly ordered or organized space structure of dislocation distribution under the action of exterior environment. The dislocation patterning is closely related both to micro-mechanical characters of materials and to specific deformation processes. As it has been well-learned, the plastic deformation in crystalline materials is controlled by the motion and multiplication of dislocations. Therefore, the study of dislocation and dislocation pattern formation will improve our basic understanding to the present micro-plasticity theory and material performance characterization.

Received 8 May 1995, revised 14 July 1995
* The project supported by the National Natural Science Foundation of China, Grant No.19392300

Up to now, a large number of works have been done for the better understanding of the behavior of a single dislocation since the Frenkel-Kontorova model and Peierls-Nabarro model were established in 1938 and 1940[3~5], respectively. But, from microscopic point of view, there are a great number of dislocations in a crystalline body and therefore, the interaction among dislocations must be taken into account, especially in the research of dislocation pattern formation. This likes a many-body problem with very complicated background. In general, there are three ways to deal with this problem, that is, the continuum dislocation field theory, the statistical mechanics of dislocations as well as the molecular dynamical simulation. However, it seems that no very essential progress has been achieved in the research of dislocation pattern dynamics based upon these three theories. In the last decade, the development of nonlinear sciences brings some new hopes to researchers of dislocation theory as briefly described below.

Early in 1970, comparing with the spinodal decomposition in phase transition, Holt[5] proposed a dynamical model to describe the formation of cell structure of dislocation patterns, and he successfully explained the relation between the cell size and dislocation density. Because the growth of dislocation density does not obey an ordinary continuity equation, the application of Holt's theory seems quite limited. In 1974, Winter[7] adopted a two-phase model in equilibrium statistical mechanics to account for the formation and evolution of persistence slide band (PBS)[4]. However, the plastic deformation process which depends on the motion of dislocations is irreversible and far away from thermal equilibrium state.

In 1985, Walgraet and Aifantis[8] first used a nonlinear dynamical method developed in nonlinear science to study the dislocation pattern formation. They considered the dislocation pattern formation as a nonequilibrium self-organization phenomenon and made use of two kinds of dislocations–the slow dislocation and the fast one–to mimic the interaction among dislocations. At one hand, they obtained abundance of results from this model and, at the other hand, however, this model could not provide a satisfactory explanation to the coexistence and the transition of the different dislocation patterns, and it can not deal with the relation between the dislocation pattern and the stress-strain curve during cyclic loading.

In 1988, Kratochvil[9] proposed a new model to connect the dislocation pattern formation to the plastic constitutive relation. Under some reasonable assumptions, this model successfully predicted the vein pattern of dislocations at early stage of fatigue process and is still in development nowadays. In addition, the cell automata technique has been used to simulate the dislocation pattern formation by Kubin, Martin, et al.,[9,10] and there is reported the occurrence of the chaotic behavior in the process of dislocation pattern formation.

In this paper, introducing the relaxation effect on dislocation density flux, the authors try to propose a new model to simulate, and therefore to explain the dislocation pattern formation. The linear stability analysis in terms of this model shows that there exists an

intrinsic wave number, which could lead to bifurcation of space structures of dislocation density. The numerical results obtained on the system of equations suggested demonstrate the coexistence and transition between different dislocation patterns. This model can also show qualitatively the stress-strain curves, multi-slip system and the formation of cell structure during deformation.

The paper will derive, at first, the governing dynamical equations on the fluctuation of dislocation density, and then, a linear stability analysis to the equations is carried out and some numerical results will be presented and the stress-strain curves will be discussed.

2 DYNAMICAL EQUATION OF DISLOCATION DENSITY

Let $\boldsymbol{B} : (B_1, B_2)$ be the vector which describes the fluctuation of dislocation density at a certain space point. Corresponding the each component B_i, $(i = 1, 2)$ there is a generalized conservation equation,

$$\partial_t B_i + \nabla \cdot \boldsymbol{J}_i = f_i(\boldsymbol{B}) \quad (i = 1, 2) \tag{1}$$

where $\boldsymbol{J}_i$ is a dislocation flux vector corresponding to B_i, and $f_i(\boldsymbol{B})$ represents nonlinear interactions among dislocations, including proliferation and annihilation of dislocations. The Eq.(1) is identical to that of Aifantis in which there are some parameters depending on the average stress, strain and temperature. To close the equations, a proper constitutive equation for the dislocation density flux is needed. In the above mentioned Holt and Aifantis' papers[8], they both suggested the constitutive equation as follows

$$\boldsymbol{J}_i = -\boldsymbol{D}_1 : \nabla B_i + \boldsymbol{D}_2 : \nabla^3 B_i \tag{2}$$

In this equation, the relaxation effect of relating the rate of flux to dislocation density gradients has been neglected. However, the relaxation effect sometimes plays an important role which should be considered in the diffusion of dislocation. Early in 1953, Crank[12] put the molecular relaxation effect into consideration on polymer diffusion. The diffusion of dislocation in crystal is reasonably supposed to be similar to that in polymer, a dislocation line corresponds to a long molecule chain of polymer. The diffusion effect is also considered in recent study on chemical diffusion-reaction dynamics[13]. Based on this consideration, we propose a new constitutive equation to the dislocation density flux, that is

$$\eta \partial_t \boldsymbol{J}_i + \boldsymbol{D} : \nabla \mu_i = -\boldsymbol{L} : \boldsymbol{J}_i \tag{3}$$

where η quantifies the relaxation time. μ_i represents the so-called "chemical potential" for the dislocated media. When η is very small and can be neglected, the Eq.13 returns to the ordinary form. As suggested by many authors, μ_i comes from the variation to the free energy functional of dislocation density, Hence, we have

$$\int \mu_i \delta B_i \mathrm{d}v = \delta \int G \mathrm{d}v \tag{4}$$

where G is the specific free energy functional of fluctuation of dislocation density, and δB_i is the variation of the i-th dislocation density. For an isothermal process, if we choose G as

$$G = g(\boldsymbol{B}) + r\sum_{\lambda}(\nabla B_i)^2 \tag{5}$$

then, through (4), μ_i can be expressed as

$$\mu_i = \frac{\partial g(\boldsymbol{B})}{\partial B_i} - p\nabla^2 B_i \tag{6}$$

If $g(\boldsymbol{B})$ is given by

$$g(\boldsymbol{B}) = -\alpha|\boldsymbol{B}|^2 \tag{7}$$

Eq.(3) becomes Eq.(2), and when $\eta = 0$ and $\alpha < 0, L > 0$, that is the case as discussed by Holt and Aifantis[6,8].

When the dislocation density fluctuation is a slow varying function of time and space,the state of the system will be determined by the minima of the free energy functional. If Eq.(7) is chosen, the minimum of the free energy functional corresponds to the state without fluctuation of dislocation density. When a dislocation pattern appears, the fluctuation of dislocation density also exists, another minimum of $g(\boldsymbol{B})$ must exist, that means that there at least exist two minima. Therefore, the simplest form of $g(B)$ may be given as

$$g(\boldsymbol{B}) = -\alpha|\boldsymbol{B}|^2 + \beta|\boldsymbol{B}|^4 \tag{8}$$

On the other hand the detail of the nonlinear term $f_i(\boldsymbol{B})$ in Eqs.(1) is not so important for the bifurcation analysis. Since zero is a homogeneous stationary solution, the following condition should be satisfied

$$\left.\begin{aligned} f_i(\boldsymbol{B}) &= \lambda_i B_i + h_i(\boldsymbol{B}) \\ h_i(\boldsymbol{B})|_{B_i=0} &= 0 \end{aligned}\right\} \tag{9}$$

Thus, the Eqs(1),(3),(4),(5),(8) and (9) form a closed system. Even if the relaxation effect is neglected, it is clear that the diffusion of dislocation does not satisfy the ordinary Fick law because diffusion coefficients are related to the fluctuation of dislocation density.

3 DISLOCATION PATTERN FORMATION

In this section, we consider a simple case: $B_2 = 0, B_1 = B$ in 2-dimension problem. Let $\boldsymbol{J}_2 = 0, \boldsymbol{J}_1 = \boldsymbol{J} = (J_x, J_y)$, the fundamental Eqs. (1) and (3) can be written as

$$\begin{aligned} &\partial_t B + \partial_x J_x + \partial_y J_y = \lambda B + h(B) \\ &\eta\partial_t J_x + D\partial_x(-2\alpha B + 4\beta B^3 - 2p(\partial_{xx} + \partial_{yy})B) = -LJ_x \\ &\eta\partial_t J_y + D\partial_y(-2\alpha B + 4\beta B^3 - 2p(\partial_{xx} + \partial_{yy})B) = -LJ_y \end{aligned} \tag{10}$$

where the parameters have reduced accordingly, $\alpha, \beta, \gamma, D, L$ and η are supposed to be all positive, L and D must also be positive to ensure a positive entropy production.

We will discuss two cases, that is, $\eta = 0$ and $\eta \neq 0$, respectively.

1) $\eta = 0$, the Eq.(10) can be reduced to a single equation for B

$$\partial_t B - \frac{D}{L}\nabla^2(-2\alpha B + 4\beta B^3) + \frac{2Dp}{L}\nabla^4 B = \lambda B + h(B) \tag{10a}$$

This is Cahn-Hilliard reaction diffusion equation. It is easy to prove that the above equation has no wave solution. The conditions for which the space dislocation pattern appears are the same as for $\eta \neq 0$

2) $\eta \neq 0$

Because zero is the homogeneous stationary solution of the equation, we have to investigate the linear stability near the zero solution. The linearized form of (10) is

$$\begin{aligned} &\partial_x B + \partial_x J_x + \partial_y J_y = \lambda B \\ &\eta\partial_t J_x + D\partial_x(-2\alpha B - 2p(\partial_{xx} + \partial_{yy})B) = -LJ_x \\ &\eta\partial_t J_y + D\partial_y(-2\alpha B - 2p(\partial_{xx} + \partial_{yy})B) = -LJ_y \end{aligned} \tag{11}$$

The Eq.(11) is assumed to take the solution in the form

$$\begin{aligned} B &= U_1 \exp(\omega t)\exp\{\mathrm{i}(K_1 x + K_2 y)\} \\ J_x &= U_2 \exp(\omega t)\exp\{\mathrm{i}(K_1 x + K_2 y)\} \\ J_y &= U_3 \exp(\omega t)\exp\{\mathrm{i}(K_1 x + K_2 y)\} \end{aligned} \tag{12}$$

By inserting Eq.(12) into the Eq.(11), the characteristic equation corresponding to Eq.(11) is obtained,

$$\begin{vmatrix} \omega - \lambda & \mathrm{i}K_1 & \mathrm{i}K_2 \\ C_1 & \eta\omega + L & 0 \\ C_2 & 0 & \eta\omega + L \end{vmatrix} = 0 \tag{13}$$

where

$$\begin{aligned} C_1 &= [2pDK_1(K_1^2 + K_2^2) - 2\alpha DK_1]\mathrm{i} \\ C_2 &= [2pDK_2(K_1^2 + K_2^2) - 2\alpha DK_2]\mathrm{i} \end{aligned}$$

The Eq.(13) can be rewritten as

$$(\eta\omega + L)\left[\eta\omega^2 + (L - \lambda\eta)\omega - \lambda L + 2D(-\alpha K^2 + pK^4)\right] = 0 \tag{14}$$

where $K^2 = K_1^2 + K_2^2$. If $\omega < 0$, there will be no space structure, so we only consider the case $\omega > 0$. For $\omega > 0$, the zero solution is unstable and the space structures will occur. For the critical value $\omega = 0$, we have

$$\lambda = \frac{2D}{L}(-\alpha K^2 + pK^4) \tag{15}$$

λ is a bifurcation parameter, the function $\lambda = \lambda(K)$ is shown in Fig.1.

When $K = K_c = \sqrt{\alpha/2p}$, there is a minimum $\lambda = \lambda_c = -\dfrac{\alpha^2 D}{2pL}$. Since both α and p are positive, there will always be a pattern-like space structure for the dislocation distribution.

The extreme values K_c and λ_c depend on α and p respectively, the following relation between λ_c and K_c can be obtained,

$$\lambda_c = -2p\frac{D}{L}K_c^2$$

This relation is shown in Fig.2.

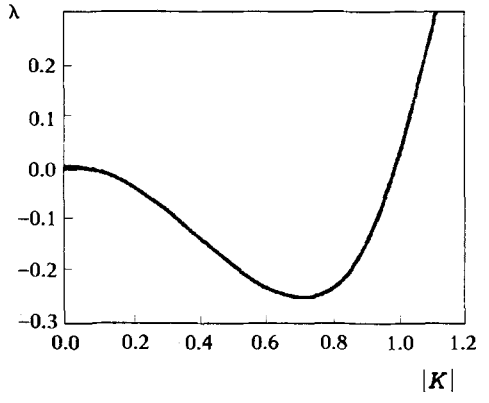

Fig.1 λ versus K

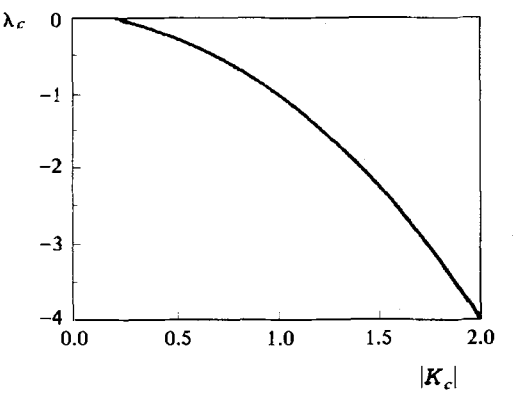

Fig.2 λ_c versus K_c

If let α be a bifurcation parameter, we have from (15)

$$\alpha = pK^2 + \frac{L|\lambda_c|}{2DK^2} \tag{16}$$

for the case $\lambda = \lambda_c < 0$. The relation (16) is shown in Fig.3.

It is clear that these is a minimum $\alpha_c = \sqrt{\dfrac{2pL|\lambda_c|}{D}}$, and another minimum $K_c^2 = \sqrt{\dfrac{L|\lambda_c|}{2pD}}$, the above two kinds of minimum conditions are equivalent.

Since $K^2 = K_1^2 + K_2^2$, there exist some degenerations of wave vector, any wave vector that satisfies $K_1^2 + K_2^2 = K_c^2$ makes λ minimum (see Fig.4). The linear analysis can not split the degeneration of the wave vectors.

Three wave vectors and the corresponding dislocation structures are considered as follows,

1) $(K_1, K_2) = (K_c, 0)$

The solution of linearized equation for the fluctuation of dislocation density is approximately

$$B \sim \sin K_c x \tag{17}$$

this could correspond to a wall structure in dislocation patterns.

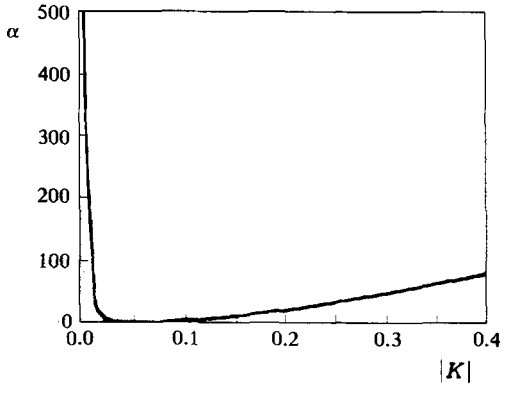

Fig.3 α versus K

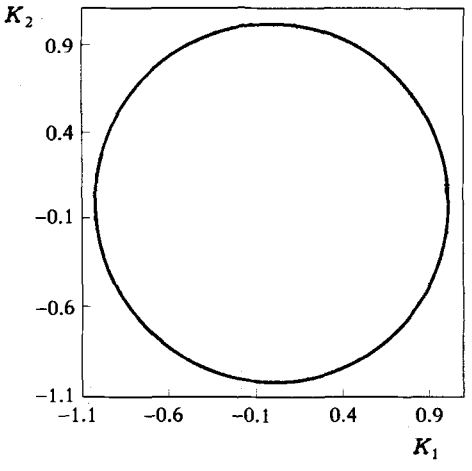

Fig.4 Wave vector degeneration

2) $(K_1, K_2) = (K_1, 0)$ and $(0, K_c)$

For this case, we have

$$B \sim C_1 \sin K_c x + C_2 \sin K_c y \tag{18}$$

where C_1 and C_2 are the two arbitrary constants, this relation corresponds a rectangular cell structure in dislocation patterns.

3) $(K_1, K_2) = K_c\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right), K_c\left(\frac{-1}{2}, \frac{\sqrt{3}}{2}\right)$ and etc.

This is a hexagonal cell structure and

$$B \sim \sin K_c\left(\frac{x}{2} + \frac{\sqrt{3}}{2}y\right) + \sin K_c\left(-\frac{x}{2} + \frac{\sqrt{3}}{2}y\right) + \cdots \tag{19}$$

when the nonlinear effect is taken into account, the above cell structures will be deformed.

It is hard to distinguish the degenerated wave vectors in linear analysis. But, with consideration in physics, the wave vector (K_1, K_2) can be chosen reasonably. As is known, the dislocation structures are related to the active slip systems in plastic deformation process, there must be a relation between wave vector and slip system, this is a very strong restriction on the selection of wave vectors.

The slip systems start to be activated when the stress exceeds a certain critical value. Since $K_c^2 = \dfrac{\alpha^2}{2p}$. K_c is determined by α as p is fixed. α is related to shearing strain in general, and in some circumstances there is a relation

$$\alpha = \alpha_0(\log\gamma - \log\gamma_c)^{2(2n+1)} \tag{20}$$

where n is a positive integer, γ_c is a critical parameter and its description will be given in the next section. As γ becomes larger, α and k_c are larger too, the corresponding dimension of the dislocation space structure becomes smaller. The cell structure appears more reasonably for large K_c.

The above analysis can not get rid of the coexistence of different dislocation patterns, but the proposed model should be able to describe this phenomenon. When $\eta \neq 0$, these is a wave motion solution, However, at present, we are not able to choose the value of η exactly. In the following section some numerical calculations are given to demonstrate the coexistence of dislocation patterns and to explain the transition from wall structure to cell structure.

4 NUMERICAL RESULT

At first, we choose nonlinear interaction function $h(B)$ in (10) as follows

$$h(B) = \lambda_1 B^2 + \lambda_2 B^4$$

then we present some numerical results of the Eq.(10). Since we deal with the evolution problem of dislocation density, both the initial conditions and the boundary conditions must be prescribed. For simplicity, we restrict the whole system on a torus and there is a periodic boundary condition available for the simulation of an infinite plane. However, to the initial conditions, there are many different choices. We consider two kinds of initial conditions. One is that there is a small fluctuation of dislocation density in a local region. The other is that the fluctuation of dislocation density is in very slow spatial variation in the whole region. Without loose of generality, η and D are set to be unity in the following numerical simulation.

The numerical skill used in solving Eq.(10) is developed from a predictor-corrector method, which is of absolute stability. The system of difference equations is solved by alternative direction implicit (ADI) method. The differential operators are approximated by a central difference scheme. To the nonlinear terms, we use a simple linearization method, that is, the old K-th values are used to replace the unknown $(K+1)$-th values in nonlinear terms. In the numerical experiment, we find that for a given time region, the Eq.(10) is sensitive to the values of parameters. For some combinations of parameters, the calculation stops due to overflow; for some other combinations of parameters, homogeneous solutions occur, for some other specific combinations of parameters, many interesting patterns appear and develop with time. This fact shows that the system is rich of bifurcation phenomena. In the following, we present three groups of the solutions with their corresponding figures.

1) The wall structure of the fluctuation of dislocation density. The parameters are selected as

$$\lambda = -0.5, \quad \lambda_1 = 0.0001, \quad \lambda_2 = 0.0001$$

$$\alpha = 100, \quad \beta = 5, \quad p = 5, \quad L = 99$$

the evolution of dislocation density is shown in Fig.5(a-i)

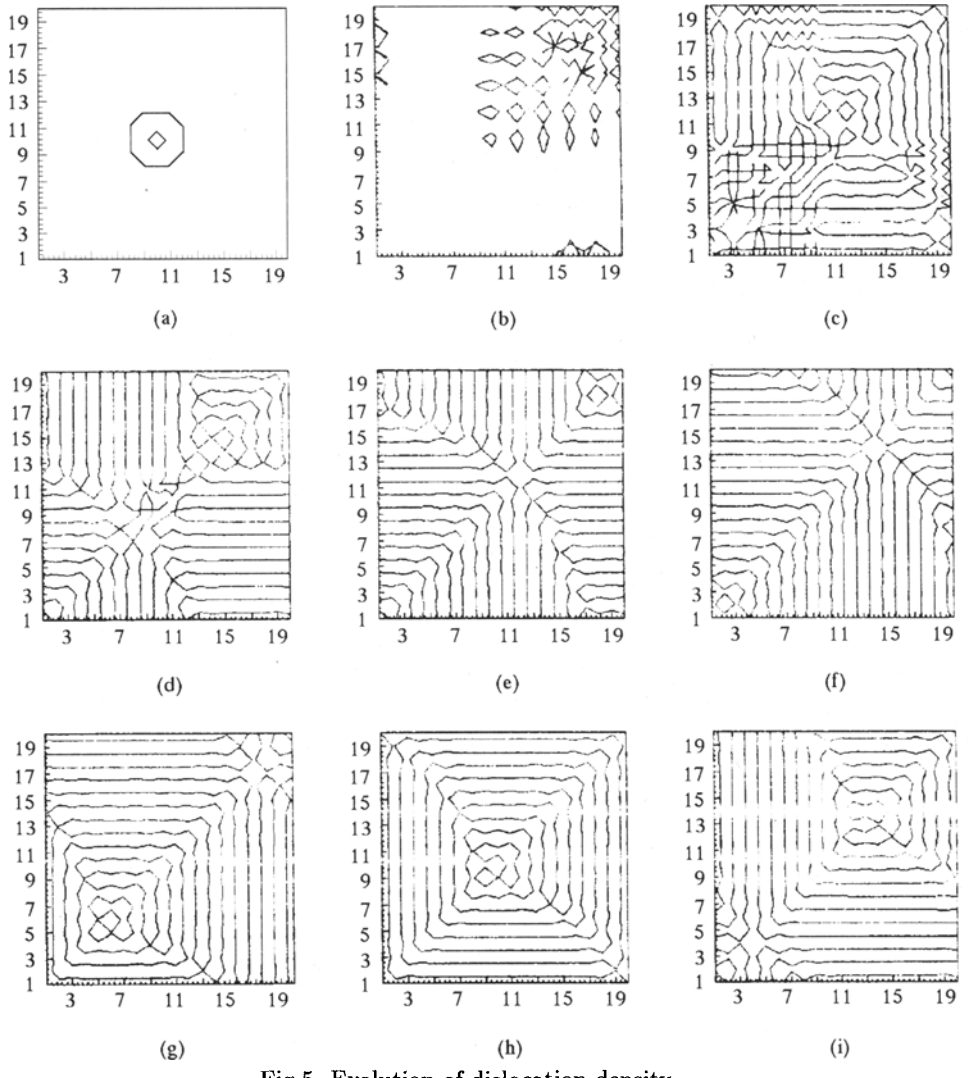

Fig.5 Evolution of dislocation density

2) The transition from wall structure to cell structure, if the parameters are chosen as

$$\lambda = -0.5 \qquad \lambda_1 = 0.11 \qquad \lambda_2 = 0.11$$

$$\alpha = 100 \qquad \beta = 35 \qquad p = 36 \qquad L = 99$$

The evolution of dislocation patterning is shown in Fig.6(a-i), taken at different times.

3) Other patterns of the fluctuation of dislocation density. If we use

$$\lambda = -0.5 \qquad \lambda_1 = 0.0001 \qquad \lambda_2 = 0.0001$$

$$\alpha = 100 \qquad \beta = 51 \qquad p = 49 \qquad L = 93$$

Then, the evolution is shown in Fig.7 (a-i), which show the complexity of dislocation pattern evolution.

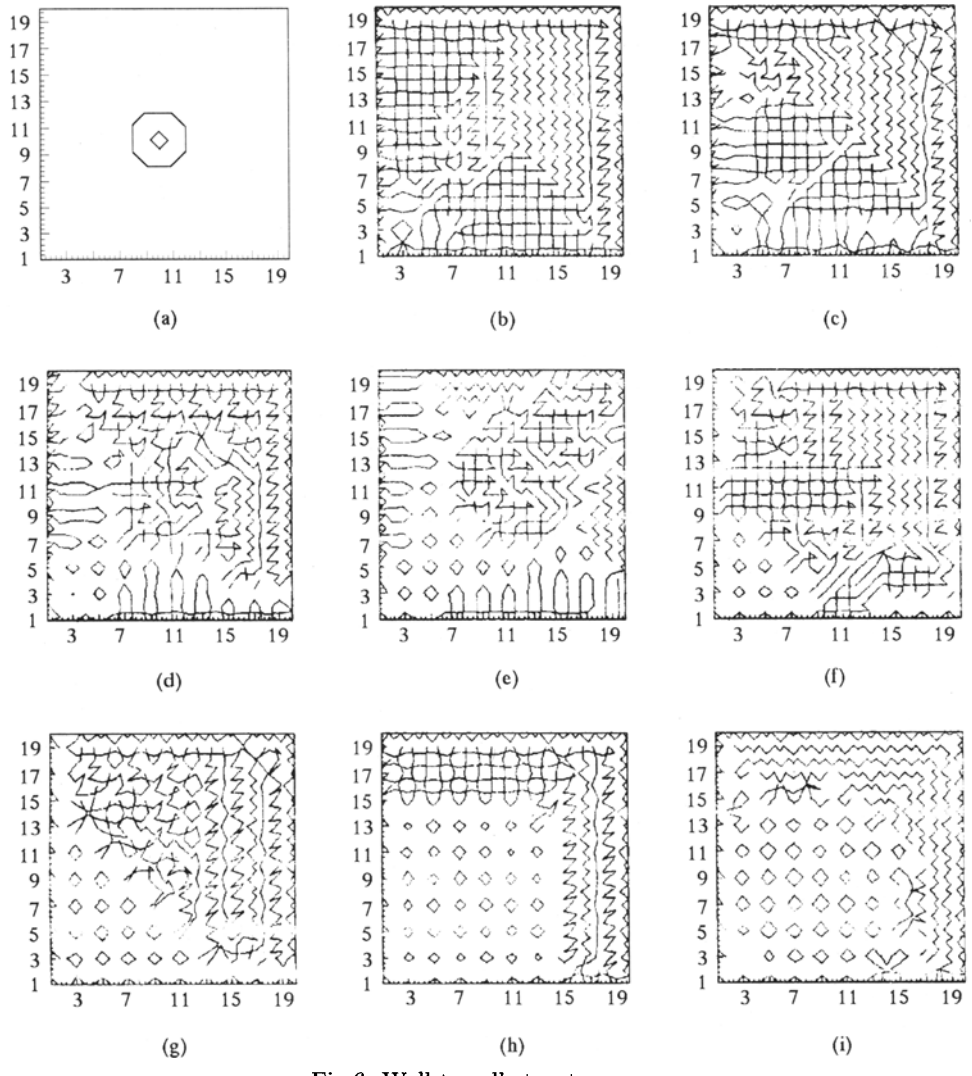

Fig.6 Wall to cell structure

From these results of the calculation, we conclude that the choices of the above parameters are different, the pattern formations and the pattern evolutions are quite different, though the initial values are the same.

Therefore, the above numerical examples illustrate that the new model is reasonable and can bring about rich phenomena in pattern formation and pattern transition.

On the stress-strain curve for cyclic loading. The total free energy of the dislocation system should be a minimum when dislocation patterns are formed. This leads to

$$\mathrm{d}g(B)/\mathrm{d}B = 0 \tag{21}$$

If the fluctuation of dislocation density varies very slowly with respect to time and to space. Since both α and β are positive, (21) has a nonzero solution except the constant solution

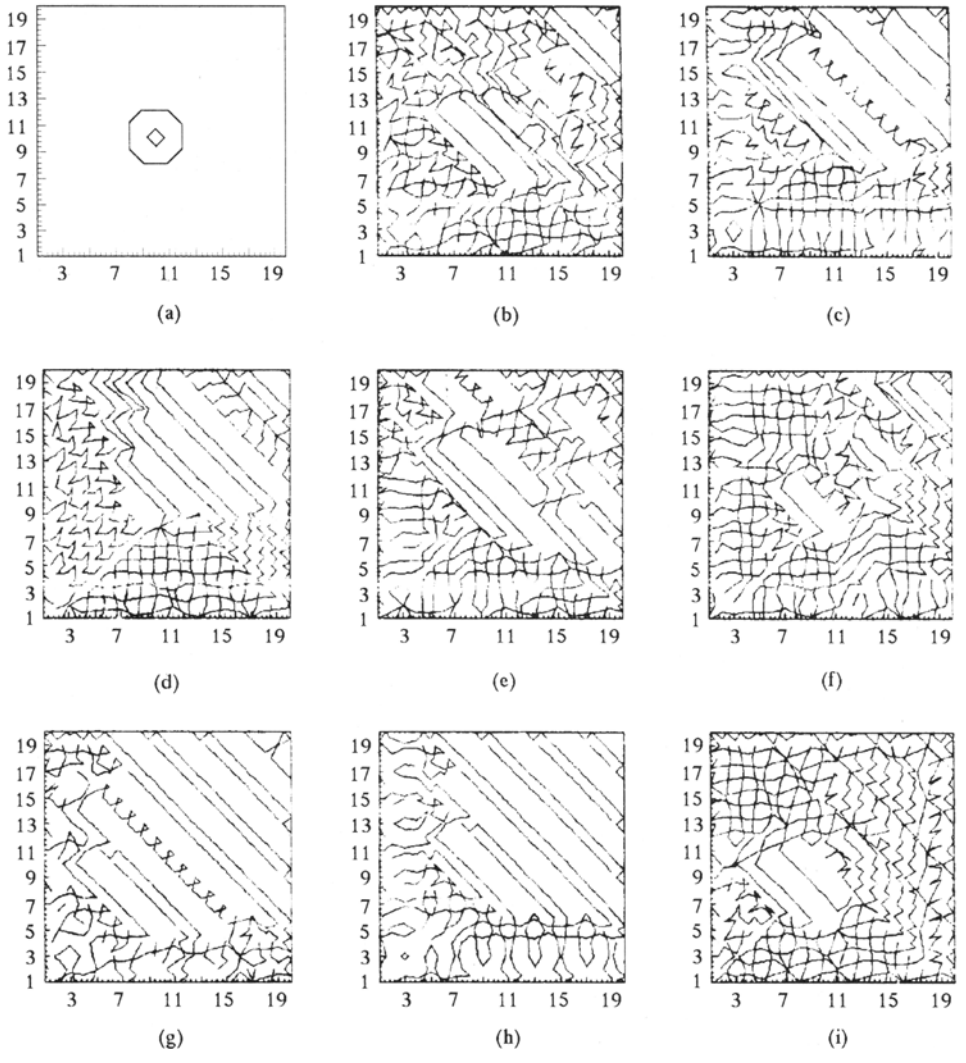

Fig.7 Complexity of dislocation structure

$$B = \sqrt{\frac{\alpha}{2\beta}} \tag{22}$$

For the empirical stress-dislocation relation

$$\sigma = K_0(B + B_0)^{1/2} \tag{23}$$

where B_0 is average initial dislocation density, B is the fluctuation of the dislocation density. By plugging the expression (20) into (23), the following stress-strain relation is obtained

$$\tau = \sigma_0[(\log\gamma - \log\gamma_c)^{2n+1} + (\log\gamma_c)^{2n+1}]^{1/2} \tag{24}$$

where B_0 is replaced by $(\log\tau_c)^{2n+1}$. The relation of (24) is illustrated in Fig.8.

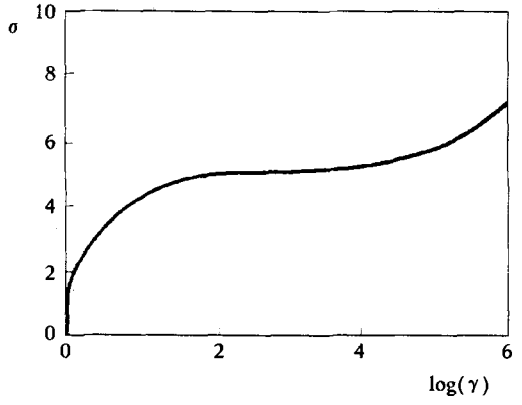

Fig.8 Stress-Strain Relation

The larger n is, the longer the horizontal part of the curve is. The relation (24) can behave in a good approximation as the stress-strain curve in cyclic loading condition.

From K_c and (22), the dimension of the dislocation pattern, $d = 2\pi/K_c$, can be expressed as

$$d = 2\pi\sqrt{\frac{8}{\beta}}\frac{1}{\beta} \tag{25}$$

The $\tau - d$ relation can be derived from (23), that is

$$\sigma = \sigma_0(2\pi\sqrt{\frac{9}{\beta}}\frac{1}{d} + B_0)^{1/2} \tag{26}$$

Only for large d, the above relation leads to linear characteristics of the stress-strain relation.

5 CONCLUSION

The dislocation patterning is one of most complicated many body phenomena. Therefore, at present it is reasonable and necessary to develop a simplified model to deal with such labyrinthine phenomena. In this paper, we adopt a new dynamic model to simulate the dislocation pattern formation. In this model, The non-Fick effect and relaxation effect of diffusion of dislocations have been considered. In the numerical experiment, It is found that the Eq.(10) of controlling the evolution of dislocation density and flux is sensitive to the selection of the values of parameters. For some combination of parameters, the calculation is stopped due to overflow, or only gives a trivial homogeneous solution. For some other particular combination of parameters, many interesting patterns occur and the transition phenomena from one pattern to another are also found. These facts show that the new model is rich of bifurcation. The stress-strain behavior under cyclic loading and the dimension of the call structure are discussed briefly. There are two important problems being left for our further study: how to relate the macroscopic state parameters to the model of dislocation pattern formation and how the bifurcation of the dislocation system bring about the chaotic

behavior. The further investigation of these problems will improve greatly our understanding to nowadays plasticity theory and enrich our knowledge to nonlinear phenomenon in material sciences.

REFERENCES

1 Qian Zhengfang, Duan Zhuping, Wang Wenbiao. Advances in dislocation patterns formation. *Advances in Mechanics*, 1993, 23(3):92 (in Chinese)

2 Kubin L P, Estrin Y, Canova G. In: Walgraef D, Ghonien N, eds. Patterns, Defects and Material Instabilities. Kluwer Acad Pub., 1990. 277~302

3 Frenkel J, Kontorova T. *Phys Z Sov*, 1938, 13: 1

4 Peierls R E. *Proc. Roy. Soc.*, 1940, 52: 23

5 Nabarro F R N. *Proc. Roy. Soc.*, 1947, 59: 256

6 Holt D L. Dislocation cell formation in metals. *J Appl Phys*, 1970, 41: 3197~3201

7 Winter A T. *Phil. Mag.*, 1974, 30: 719

8 Walgraef D, Aifantis E C. Dislocation patterning in fatigued metals as a results of dynamical instabilities. *J Appl Phys*, 1985, 58: 688~691

9 Kratochvil J. Dislocation pattern formation in metals. *Revue Phys. Appl.*, 1988, 23:419~429

10 Kubin L P, Lepinoux J. The Dynamic Organization of Dislocation Structures. In: Kettunen PO, Lepistö TK, Lehtonen ME, eds. Strength of Metals and Alloys (ICSMA-8), Vol.1. Oxford: Pergaman Press, 1988: 35~59

11 Martin G, Kubin L. Nonlinear Phenomena in Material Sciences. Aedermannsdorf, CH: Trans. Tech. Publications, 1992,

12 Crank J. *J. Polymer Sci.*, 1953, 1:151

13 Cho Ung-In and Eu B C. Ayperbolic reaction-diffusion equations and chemical oscillations in the Brusselator. *Physica*, 1993, D68: 351~363