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Author(s)	Shoji, Tetsuya; Miura, Seiji; Mohri, Tetsuo
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Reaction-Diffusion Equation for Dislocation Multiplication Process *1

Tetsuya Shoji *2, Seiji Miura and Tetsuo Mohri

Division of Materials Science and Engineering, Graduate School of Engineering, Hokkaido University, Sapporo 060-8628, Japan

In order to take multiple behavior of both mobile and immobile dislocations into account, Reaction-Diffusion equation is employed and a stress-strain curve is calculated. Characteristic three stages of a stress-strain curve are reproduced. The serration observed in the early stage of the deformation is interpreted based on the microscopic inhomogeneous multiplication process of dislocations leading to self-organization.

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1. Introduction

In order to describe the *collective behavior of dislocations*, one must consider various aspects of dislocation reactions, such as dynamic recovery, immobilization (mobilization) of mobile (immobile) dislocations, multiplication, *etc.*, leading to evolution/devolution of dislocation density. In most of the former works, however, we notice short-comings that the description of immobile dislocations is not sufficient and, therefore, one can hardly reproduce a subtle feature of stress-strain curve such as transient behavior associated with a sudden change of deformation condition.[1)]

Among various theoretical tools, one possible way to incorporate immobile dislocation behavior is to employ Reaction-Diffusion equation (hereafter R-D equation) which has been developed to study spatio-temporal pattern formation[2)] arising from non-linear couplings of elementary reactions which is a characteristic feature of *far-from-equilibrium* phenomena. Body of the applications of R-D equation is centered around pattern formation in non-linear chemistry and fluid dynamics, but the power and versatility of R-D equation have been gradually recognized in the study of dislocation dynamics[3,4)] which is, in fact, highly far-from-equilibrium phenomenon associated with energy dissipation. In general, R-D equation consists of two parts, diffusion term and reaction terms. In the present context, the diffusion term represents movement of dislocations through the material and various dislocations reactions are considered in the reaction terms which play a key role in describing mobilization and immobilization processes.

In this study, two R-D type partial differential equations are formulated in order to describe the time evolution behavior of both mobile and immobile dislocation densities. These equations are coupled in the reaction terms through immobilization (mobilization) of mobile (immobile) dislocations. The simultaneous equations are solved for a continuum which is divided into a series of segment, which enables one to analyze microscopic non-uniform deformation process. Then, by combining with a constitutive equation, a stress-strain curve is calculated. Thereby, the present study based on R-D equation is expected to provide detailed insight of collective behavior of dislocations along a calculated stress-strain curve.

2. Calculation Model

2.1 Evolution equation of dislocation density

During the plastic deformation, dislocation distribution undergoes complex microscopic processes and evolves/devolves with time. In the present study, the evolution of mobile and immobile dislocation densities are formulated in a separated manner with two R-D equations. Mobile dislocations participate in plastic deformation by a slip on the glide plane, while immobile dislocations hinder and capture the moving dislocations. Immobile dislocations consist mainly of two types; the first type is a forest dislocation which is in the secondary slip system, and the second type is a mobile dislocation which is pinned on the primary slip system by forest dislocations and can be mobilized with the aid of effective stress.

Not only pinning and freeing processes discussed above, also multiplication and recovery processes as well as diffusion process should be taken into account in the R-D equations. Described below are the details of five physical processes involved in the R-D equations of the present study.

2.1.1 Diffusion

During plastic deformation, dislocations move through neighboring segments by a slip (mobile dislocation) and a climb (immobile dislocation) motions. Such a movement of dislocations can be expressed as an effective diffusion process.[5)] It is pointed out that, for mobile dislocations, one needs to distinguish two types of dislocations depending upon the sign of Burgers vector with reference to the direction of applied stress. Following the prescription of Walgraef *et al.*,[6)] it is found that the diffusion coefficient for mobile dislocation is not constant as will be seen in eq. (2).

2.1.2 Pinning

The pinning of mobile dislocations by immobile dislocations is originated from the trapping by the interaction field of latter dislocations. The mathematical expression of this process is not transparent, thus a series expansion in terms

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*2Graduate Student, Hokkaido University.

of $p_n N_m N_i^n$ ($n = 1, 2 \cdots$) is adopted, where p_n is a pinning rate[5] and N_m is a mobile dislocation density. In order to avoid numerical complexity, we confine ourselves only to $n = 2$ in the present study and, hereafter, the explicit dependencies on n is neglected.

2.1.3 Freeing

The mobilization of immobile dislocations takes place with the help of effective stress. This is due to a destruction of dipole and decapturization from forest dislocations. The occurrence of this process is proportional to the effective stress, therefore, the term $f\tau_e N_i$ is incorporated[7] in the equation where f and τ_e are freeing rate of immobile dislocations and effective stress, respectively.

2.1.4 Multiplication

Multiplication process of immobile dislocation is caused by intersection between mobile and immobile dislocations. This process is proportional to both the area swept by mobile dislocations and the number of immobile dislocations encountered in a unit area. The multiplied length per each intersection is roughly in the order of the magnitude b of Burgers vector and the term $Abv_m N_m N_i$ is incorporated in the R-D equation with $10^0 \sim 10^1$ for a constant A and v_m is the average velocity of mobile dislocations.

2.1.5 Recovery

A dynamic recovery process of dislocations takes place when dislocations with opposite sign encounter. This process is considered only for immobile dislocations and the rate of annihilation is proportional to the product of density, velocity of immobile dislocations and a constant r which characterizes the critical length of annihilation and depends on the type of dislocations. Hence one expresses recovery process by $rv_i N_i^2$ [7] where v_i is a climb rate of immobile dislocations. This process is neglected for mobile dislocations due to negligible contribution as compared with other processes.

Based on these considerations, two evolution equations for each type of dislocation are formulated as follows

$$\frac{dN_i}{dt} = D_i \frac{\partial^2 N_i}{\partial x^2} + p \cdot N_m \cdot N_i^2 - f \cdot \tau_e \cdot N_i + A \cdot b \cdot v_m \cdot N_m \cdot N_i - r \cdot v_i \cdot N_i^2 \quad (1)$$

$$\frac{dN_m}{dt} = \nabla \frac{v_m}{p \cdot N_i^2} (\nabla v_m \cdot N_m) - p \cdot N_m \cdot N_i^2 + f \cdot \tau_e \cdot N_i. \quad (2)$$

Note that the order of the right hand side of both equations corresponds to that of the descriptions of physical processes 2.1.1–2.1.5 above.

2.2 Stress-strain constitutive equations

A single crystalline specimen is divided into series of segments. Each segment is regarded as a continuum which deforms uniformly and obeys the following equations.[8]

First of all, a plastic strain rate, $\dot{\varepsilon}^j$ of each segment j is given by the Orowan's relation

$$\dot{\varepsilon}^j = N_m^j \cdot v_m^j \cdot b. \quad (3)$$

Secondary, an applied stress τ_a is equally loaded to all segments, thus, effective stress τ_e^j at segment j is given as,

$$\tau_e^j = \tau_a - \tau_{in}^j, \quad (4)$$

where τ_{in}^j is an internal stress caused by immobile dislocations written as

$$\tau_{in}^j = \frac{\mu \cdot b}{\beta} N_i^{1/2}, \quad (5)$$

where β is a constant describing the magnitude of interaction between dislocations and μ is a shear modulus of the specimen. Note that the dependencies of internal stress on segment j is originated from spatial inhomogeneity of immobile dislocations. In order to avoid unnecessary complications, however, the superscript j is not explicitly indexed to N_i. Thirdly, for the dependence of mobile dislocation velocity on the effective stress, following expression of Gilman and Johnston based on experimental observation[9] is adopted,

$$v_m = v_0 \cdot \tau_e \exp\left(-\frac{Q}{k_B T}\right), \quad (6)$$

where v_0 is a constant determined experimentally, Q, k_B and T are, respectively, an activation energy, Boltzmann constant and the absolute temperature. Finally, in order to assure the compatibility between segments, we incorporated the following back stress term originally proposed by Lebyodkin *et al.*,[10]

$$\sigma_{back} = k((\varepsilon^{j-1} - \varepsilon^j) + (\varepsilon^{j+1} - \varepsilon^j)), \quad (7)$$

where k designates the strength of the spatial coupling between segments and its magnitude is in the same order of the shear modulus μ.

As a constitutive equation to describe the stress and displacement relationship, the following conventional equation[8] is adopted,

$$\frac{d\tau_a}{dy} = \frac{K \cdot S_f}{C}\left(1 - \frac{l_0 \cdot S_f \cdot \dot{\varepsilon}}{S_c}\right), \quad (8)$$

where y is the displacement of the cross-head, S_c a cross-head speed, K the rigidity of the machine-sample system, S_f the Schmid factor and C and l_0 are, respectively, the cross sectional area and the gauge length of the sample at the initial state. In calculating a stress-strain curve, the strain rate of each segment given by eq. (3) is averaged out over an entire specimen,

$$\dot{\varepsilon} = \frac{1}{N}\sum_{j=1}^{N} \dot{\varepsilon}^j, \quad (9)$$

where N is the total number of segments, and eq. (9) is substituted into eq. (8).

3. Results and Discussion

As mentioned in the previous section, one of the main concerns of the present study is to calculate a stress-strain curve. By solving a set of constitutive equations discussed above, one obtains a stress-strain curve as shown in Fig. 1. Note that both applied and effective stresses are normalized with respect to, τ_{ly}, the lower yield stress. Parameters and constants employed in this study are tabulated in Table 1. Among these parameters, Aluminum is adopted to specify materials param-

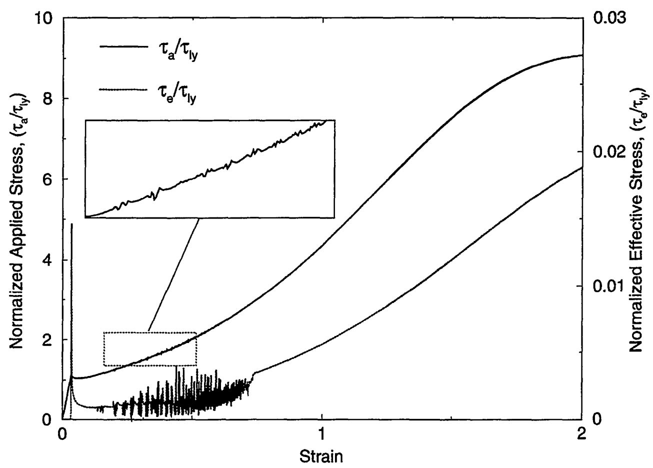

Fig. 1 Calculated stress-strain curve. Solid and dotted lines represent applied stress and effective stress, respectively. Vertical axis indicates applied (left hand side) and effective (right hand side) stresses which are normalized with respect to lower yield stress. The horizontal axis represents strain.

Table 1

Parameters and constants	Values
b	2.8635×10^{-10} (m)
μ	2.8×10^{10} (Pa)
v_{m0}	1.0×10^{-1} (m/s)
v_i	2.0×10^{-6} (m/s)
β	3.3
S_f	0.4
K	1.0×10^{3} (Pam)
S_c	1.0×10^{-5} (m/s)
l_0	1.0×10^{-2} (m)
C	1.0×10^{-6} (m^2)
f	4.0×10^{-1} (/Pas)
p	5.0×10^{-20} (m^4/s)
r	8.5905×10^{-9} (m)
A	2.0
D_i	3.0×10^{-12} (m^2/s)
Q	1.73×10^{-21} (J)
k_B	1.38×10^{23} (J/K)
T	298 (K)

eters[11)] such as burgers vector b and rigidity μ, for a spurt-like motion of a dislocation assumed in the previous section holds for a fcc-based metal and alloys. A typical experimental situation is simulated to chose external values such as rigidity of a machine-sample system K, cross-head speed S_c, and initial dimensions of a specimen C and l_0. Also, for parameters describing a slip system such as Schmid factor S_f and β, conventionally accepted values are specified. Various coefficient terms appearing in R-D equations are key to the analysis. In view of the subtle stability problems involved in the highly nonlinear character of R-D equation, most coefficient terms are directly adopted in the pioneering studies of Walgraef,[6,7)] thereby we attempted to avoid facing numerical complexities. This is believed to be accepted as an initial phase of investigation, but we do point out that further critical evaluations of parameters are indispensable particularly in connection with stability analysis.

In Fig. 1, one distinguishes three regions of the stress-strain curve, namely easy glide region in which deformation progresses comparatively at small stress, linear hardening region where the flow stress increases rapidly with strain and parabolic hardening region which results from dynamical recovery and work hardening rate decreases as strain increases. A noteworthy feature is a jerky flow magnified in the inset in Fig. 1. A jerky flow has been generally known as the consequence of a discontinuous deformation termed as Luders band deformation. It is, however, emphasized that the Luders band deformation is observed only in a poly crystal while the present calculation is attempted on a single crystal characterized by a single Schmid factor throughout the segments. Hence, in order to distinguish it from the conventional discontinuous flow, we call this process as *propagative deformation*. In the following discussion, we focus on the physical origin of the propagative deformation in terms of self-organization[12,13)] process of dislocations which is a peculiar feature expected from R-D equation.

Shown in Fig. 2 is the magnified view of the early stage of stress-strain curve where the jerky flow is observed. The spatial distributions of effective stress (dashed line) and mobile and immobile dislocations along the stress-strain curve in Fig. 2 are demonstrated in Figs. 3(a)–(d). Note that figures (a)–(d) correspond to strains specified by arrows (a)–(d) in Fig. 2, respectively. The propagative deformation process referred in Figs. 1 and 2 can be interpreted as follows. At first, one segment with low density of immobile dislocations which is in the middle segment of the specimen in Figs. 3 initiates deformation. Then, after sufficient amount of deformation of the segment, with the progress of work hardening the neighboring segments start yielding. This process is repeated until the propagation of deformation terminates at the edge of the specimen. In fact, at $\varepsilon = 0.1$ (Fig. 3(b)), the homogeneous distribution of effective stress at the initial stage (Fig. 3(a)) becomes heterogeneous. It is seen that the homogeneous stress level goes down and the effective stress τ_e at the central segment becomes zero, indicating no deformation,

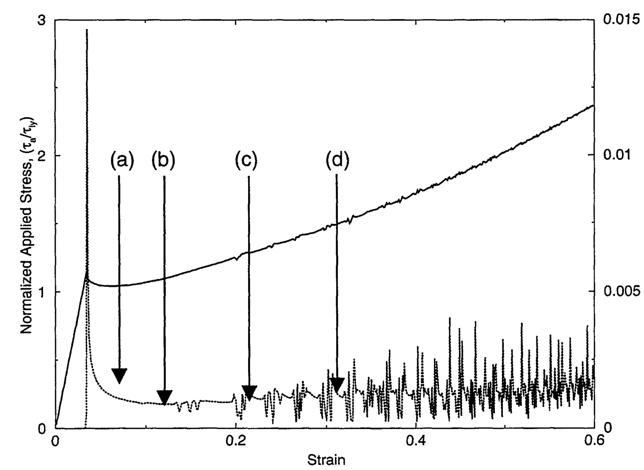

Fig. 2 Magnification of early stage of stress-strain curve in Fig. 1. (a), (b), (c) and (d) correspond to strains at 0.05 (5%), 0.1 (10%), 0.2 (20%) and 0.3 (30%), respectively.

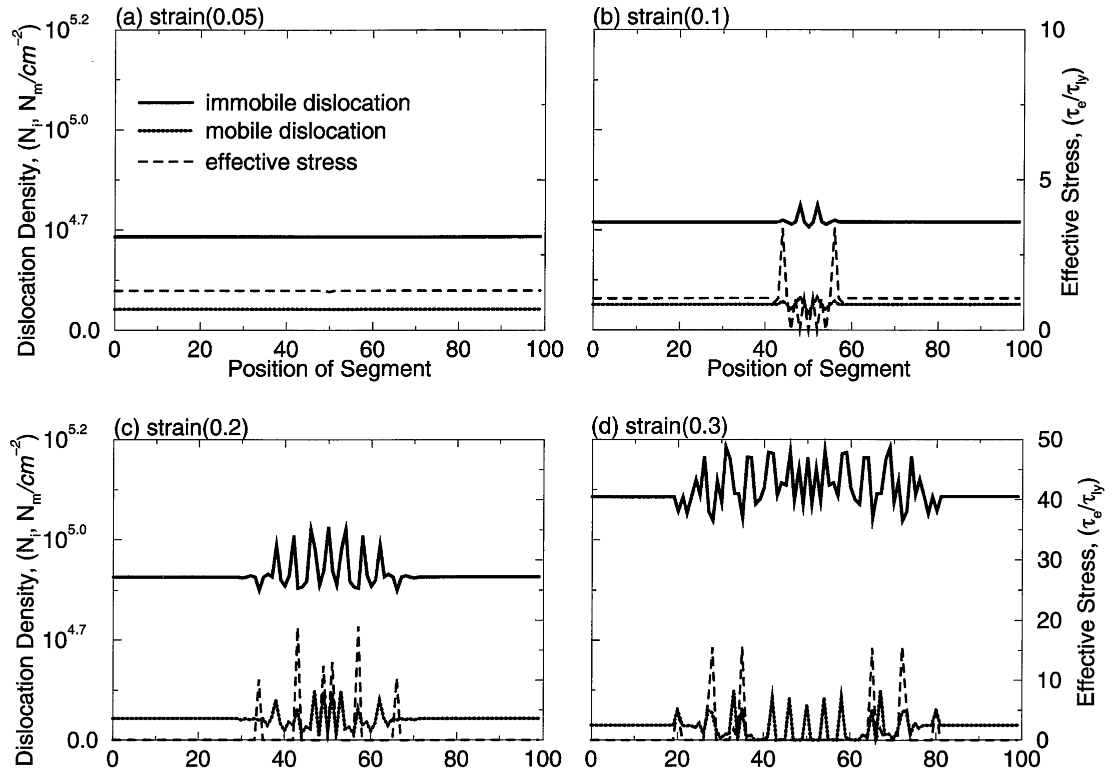

Fig. 3 Distributions of effective stress, mobile and immobile dislocation densities in 100 segments of a specimen. (a), (b), (c) and (d) correspond to strains at 0.05 (5%), 0.1 (10%), 0.2 (20%) and 0.3 (30%), respectively.

while in the neighboring segments higher effective stress induces significant deformation. At $\varepsilon = 0.2$ (Fig. 3(c)), most segments undergo no deformation and high effective stress in the center suggests the strong localized deformation of corresponding segments. Such a sequence of microscopic deformation behavior is reflected in the occurrence of the sequence of burst-type effective stresses in Figs. 3(a) to (d). Thereby, one sees that the initial homogeneous distributions of both mobile and immobile dislocations are destabilized and spatially heterogeneous patterns are formed with the progress of deformation. This is the self-organization.

In the present report, we demonstrated that the description of the evolution of dislocation densities based on R-D equation not only yields a stress-strain curve but also provides microscopic insight of multiplication process. Together with the details of stability analysis, the self-organized dislocation patterns are reported in the forthcoming publication.[12]

4. Conclusion

Based on R-D equations formulated for mobile and immobile dislocations, a stress-strain curve is calculated and microscopic multiplication process is investigated along the obtained stress-strain curve. The main feature of the stress-strain curve such as the existence of three distinctive stages are reproduced in the present calculation. In addition, it is observed that a homogeneous distribution of dislocations in the initial stage is destabilized and heterogeneous pattern formation is taken place. Such an analysis of spatio-temporal dislocation pattern formation is a unique feature endowed with the R-D equation.

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