SIMULATION OF DYNAMIC STRAIN AGING PROCESS AT THE MICROSCOPIC SCALE BY MONTE CARLO DYNAMIC MODEL

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A two-dimensional Monte Carlo dynamic model has been developed to simulate the interaction between mobile dislocations and solute atoms. When there was a single dislocation with a constant stress rate, the dislocation was pinned under low stress rate conditions, moved continuously under high stress rate conditions, and moved intermittently at an intermediate stress rate, where the step-shaped curve of dislocation displacement showed dynamic strain aging. Under multi-dislocation unstressed conditions, the solute atoms gathered below positive dislocations and above negative dislocations. Under the multi-dislocation conditions with constant stress, the dislocation displacement became longer with increasing stress. Under multi-dislocation conditions with constant stress rate, the collective pinning and unpinning results showed a step-shaped curve of total dislocation displacement. The simulation results present a microscopic view of the pinning and unpinning in dynamic strain aging.

KEY WORDS: dynamic strain aging, Portevin–Le Chatelier effect, kinetic model, dislocation motion, diffusion

1. INTRODUCTION

In a certain range of strain rates and temperatures, a special plastic instability during deformation of many alloys manifests itself by serrated stress flow in the temporal domain and strain localization in the spatial domain, which is called the Portevin–Le Chatelier (PLC) effect (Deschamps et al., 2013; Fu et al., 2012; Casarotto et al., 2009; Franklin et al., 2001; Kubin and Estrin, 1985). To date, the microscopic mechanism of the PLC effect is widely known as dynamic strain aging (DSA), i.e., the interaction between solute atoms and mobile dislocations (Zhang and Picu, 2009; Curtin et al., 2006; Fressengeas et al., 2005). During dislocation motion, solute atoms will diffuse to mobile dislocations and produce an additional pinning that causes the increment of stress. When the mobile dislocation overcomes the pinning of solute atoms by thermal activation, stress is reduced. The repeated pinning and unpinning processes result in a serrated stress curve.

Experimentally, research on the PLC effect has focused mainly on analysis of the serrated stress response (Park and Niewczas, 2008; Jiang et al., 2006), observation of the spatial PLC band (Fu et al., 2015; Zhang et al., 2005), and some qualitative or quantitative explanations combining DSA and macro results. By simulation, the models can be divided into three types. First, the dislocation transition model (Sahoo and Ananthakrishna, 1982) considers the stress variation during the transition of different kinds of dislocations. Second, the solute concentration model (Jiang et al., 2007) considers the influence of variations of the solute concentration on stress. Third, the comprehensive model (Hu et al., 2012; Lebyodkin et al., 2000) considers the combined influence of the two aforementioned mechanisms on stress. All of these models can reproduce the serrated stress curve, and some can also reproduce the propagation of a spatial PLC band. However, the simulation results are macroscopic phenomena, which do not involve processes at the microscopic scale. Some of these models do involve microscopic elements statistically by the macroscopic parameters, such as the dislocation density, solute atom concentration, etc., but do not simulate the specific process.
at the microscopic scale. Because of the limitation of experimental techniques, the microscopic DSA process, i.e., pinning and unpinning between mobile dislocations and solute atoms, still cannot be directly observed by experimental instruments. A description of the pinning/unpinning process at the microscopic scale by simulation will immensely enhance the comprehension of the PLC effect and DSA.

Therefore, using Monte Carlo methods, Wang et al. (2000) simulated the interaction between a single positive edge dislocation and a certain concentration of solute atoms. It was observed that solute atoms gather below the dislocation under the unstressed condition. At different constant shear stresses, the features of dislocation motion were different. At low shear stress, solute atoms gather around the dislocation, but at high shear stress, no such gathering occurs. The results showed the microscopic differences in the presence or absence of DSA. In physical material the dislocations are clustered and the shear stress varies in tension. The investigation on the interaction between multiple dislocations and solute atoms at constant shear stress rate is closer to the tension of the physical material.

In this study, we simulated a single dislocation’s motion at constant stress rate using Monte Carlo methods. Then, the model was extended to multi-dislocation processes, and the interactions between solute atoms and dislocations under unstressed, constant stress, and constant stress rate conditions were simulated.

2. SIMULATION METHOD

The simulation cell is a two-dimension model, as shown in Fig. 1. The unit of length in the cell is the Burgers vector amplitude, $b$. The number of dislocations and solute atoms in the cell are $N_d$ and $N_s$, respectively. Their corresponding concentrations are $\rho_d = N_d/(WH)$ and $C_s = N_s/(WH)$. In the model, only substitutional solute atoms and edge dislocations are considered. The dislocation length is denoted as $L$ with the slip direction along the $x$ axis, and the Burgers vector of dislocation is represented as $sb$ (where $s = \pm 1$ denotes the dislocation symbol). The system energy, $E$, can be divided into the work energy of shear stress, $E_1$; the interaction between dislocations and solute atoms, $E_2$; and the interaction between dislocations, $E_3$.

When a dislocation moves a distance of $\Delta x$ in response to shear stress $\tau$, the energy change (work) associated with the dislocation glide is $\Delta E_1 = -\tau sbL \Delta x$. The strain energy between a dislocation and a solute atom is defined as $E_2 = P \Delta V$, where $P$ is the hydrostatic pressure caused by the dislocation stress field and $\Delta V$ is the volume change formed by the solute atom. The specific expressions (Nabarro, 1952) are

FIG. 1: Schematic of the simulation cell ($W$ and $H$ are the width and height of the cell, respectively; $\tau$ is the shear stress; the black dot denotes the solute atom; the red, upward triangle denotes the positive edge dislocation; and the blue, downward triangle denotes the negative edge dislocation)
where $P$ is the shear modulus; $\nu$ is the Poisson ratio; $x$ and $y$ are the relative coordinates from the solute atom to dislocation; $R_s$ is the atomic radius of the solute atom; and $R_b$ is the atomic radius of the matrix.

When a dislocation moves a distance of $\Delta x$, the interaction between itself and other reference dislocations can be defined as $\Delta E = \sum F_x \Delta x$. The force $F_x$ between the moving dislocation and a reference dislocation on the glide direction in the unit length is (Hirth and Lothe, 1982)

$$F_x = \frac{s_1 s_2 \mu b^2 x (x^2 - y^2)}{2\pi (1 - \nu) (x^2 + y^2)^2}$$

where $s_1$ and $s_2$ are the symbols of two dislocations, respectively; and $x$ and $y$ are the relative coordinates from a moving dislocation to the reference dislocation. If an element (dislocation or solute atom) in the cell moves, the variation of total system energy, $\Delta E = \Delta E_1 + \Delta E_2 + \Delta E_3$, will be changed. If $\Delta E$ is less than or equal to zero, the movement is accepted. Otherwise, the movement is not accepted and the position of the element remains unchanged.

Some assumptions are made in the simulation. Isotropic material is assumed. Multiplication, annihilation, and climb of dislocation are suppressed. Interactions among solute atoms and their self-segregation are ignored. Each cell point is occupied by one solute atom or one dislocation at one time. Periodic boundary conditions are adopted. After solute atoms move across the border, they randomly distribute in the cell again. In the single dislocation simulations, when the dislocation moves across the right border, it reappears at the center of the new cell. The distribution of solute atoms relative to dislocation on the left side of the new cell is consistent with the right side of the original cell. Meanwhile, the number of solute atoms in the right side of the new cell remains consistent with the left side of the original cell, but their positions are randomly distributed. When the dislocation moves across the left border, the situation is similar. In the multi-dislocation simulation, when the dislocation moves across the border it will re-enter the cell at the opposite border.

In a physical material, dislocations and solute atoms move simultaneously with different velocities. In Monte Carlo simulations, only one element can be chosen to move a unit length at a time (step). Thus, a parameter $M$ is introduced to show the ratio of the movement rate of a dislocation to a solute atom. The total movement rate ratio for dislocations and solute atoms is defined as $M_t = N_d M / N_s$. In this simulation, the following parameters are used: $\mu = 25$ GPa; $b = 0.285$ nm; $R_b = 0.134$ nm; $R_s = 0.160$ nm; $L = 100b$; $C_s = 0.5\%$; $\nu = 0.33$, according to Al–Mg alloys; and $M = 100$ (Wang et al., 2000). The simulation time is defined by the Monte Carlo step (MCS), or $1/\Gamma$.

3. RESULTS AND DISCUSSION

3.1 Single Dislocation: Constant Stress Rate

In the simulation, the stress rate $\dot{\tau}$ is a constant value, and the simulation parameters are set as $W = 1000b$, $H = 100b$, $N_s = 500$, and $C_s = 0.5\%$, which is a similar condition to the saturated solubility of Mg in the Al matrix at room temperature. Without considering dislocation climb, the dislocation will only move along the $x$ axis. We can shrink the height of the cell to reduce the calculation. The dislocation motions at different stress rates are shown in Fig. 2. In the same simulation steps, when the stress rate is small ($5 \times 10^{-8}$ $\mu \Gamma$), the dislocation displacement is as short as 23$b$, and the dislocation is predominantly static, as shown in Fig. 2(a). When the stress rate is large ($5 \times 10^{-6}$ $\mu \Gamma$), dislocation motion is continuous with saturated speed ($16\Gamma$), as shown in Fig. 2(b). Even at the same stress, dislocation motions are different at different stress rates. As shown in Fig. 2(c), at equal stress, the dislocation is static at the low stress rate and the dislocation is kinetic at the high stress rate. This shows that in these two cases, the stresses required to start the dislocation are different. In these simulations, the dislocation resistance only arises from solute atoms gathering together; that is to say, the pinning strengths by solute atoms are different in the two aforementioned circumstances. At the low stress rate ($5 \times 10^{-8}$ $\mu \Gamma$), more time is needed to achieve the same stress, which allows more solute atoms to diffuse to the dislocation, and the dislocation is arrested by the pinning effect of solute atoms. At the high
stress rate ($5 \times 10^{-8} \mu \Gamma$), the time to achieve the same stress is shorter, causing fewer solute atoms to diffuse to the dislocation, and solute atoms cannot pin the dislocation. When the stress rate is at an intermediate value ($5 \times 10^{-7} \mu \Gamma$ or $7 \times 10^{-7} \mu \Gamma$), dislocation motion shows a characteristic step-shaped behavior, and its performance is consistent with repeated pinning and unpinning in DSA. One should note that although the dislocation motion resembles a step shape in Fig. 2(a), the dislocation only moves $23b$. This feature is closer to creeping rather than pinning and unpinning in DSA. It can be concluded from the simulation results that the dislocation is pinned by solute atoms at a low stress rate, but the dislocation is not pinned (continuously in motion) at a high stress rate. Only at the proper intermediate stress rate does dislocation motion feature pinning and unpinning. This suggests that DSA only occurs under certain conditions, in agreement with macro-scale experiments on changing strain rate. It should be noted that the simulated results are influenced by parameter $M$. Increasing $M$ can be considered as increasing the mobility of dislocations or decreasing the mobility of solute atoms. A larger $M$ value makes it more difficult for solute atoms to gather near the dislocation and easier to move the dislocation under a certain stress rate. The stress rate for a step-shaped curve
of dislocation displacement would become lower. Compared with the experiment, parameter $M$ should increase with either increasing strain rate or decreasing temperature.

### 3.2 Multiple Dislocations: Unstressed

To simulate a physical material closely, this study simulated the gathering of solute atoms to multi-dislocation under the unstressed condition. The simulation parameters are set as $W = 1000b$, $H = 1000b$, $N_s = 5000$, and $N_d = 50$. Accordingly, $C_s = 0.5\%$ is consistent with the constant stress rate condition, and $\rho_d = 6 \times 10^{10} \text{ cm}^{-2}$ approximates the dislocation density in Al–Mg alloys (Kubin and Estrin, 1990). The solute atom gathering process is shown in Fig. 3. The solute atoms are randomly distributed at the initial time. As time elapses, the solute atoms gather below the positive and above the negative dislocations, respectively. After the time of $5 \times 10^5$ MCS, the distribution of solute atoms stabilizes. This can be regarded as the aging process of the material in the static state.

**FIG. 3:** Distribution and gathering process of solute atoms in the unstressed condition at: (a) the initial time; (b) $3 \times 10^5$ MCS; (c) $5 \times 10^5$ MCS; (d) $7 \times 10^5$ MCS
3.3 Multiple Dislocations: Constant Stress

In the unstressed state, dislocations are stationary. The next simulation was of dislocation motion under a constant stress condition. The results are shown in Fig. 4 using the same simulation parameters as in Section 3.2. At low stress [Fig. 4(a)], the total displacement of dislocation motion is short and finally stabilizes, which can be interpreted as dislocations transitioning from gliding to being pinned by solute atoms. When stress increases, the total dislocation motion displacement also increases. At high stress [Fig. 4(b)], dislocation motion is continuous. Dislocations need more solute atoms to be pinned, but the dislocation motion is continuous with a velocity greater than the diffusion speed of the solute atoms, minimizing the number of solute atoms gathered around the dislocation. When dislocation motion transitions from mobile to static, the stress is less than the stress required to restart dislocation motion. When the dislocation is static, owing to the constant stress and solute atom gathering to dislocation, the force required to restart dislocation motion increases, causing the dislocation to remain static. In this case, only the dislocation pinning will appear but unpinning cannot occur.

3.4 Multiple Dislocations: Constant Stress Rate

The simulation results for multiple dislocations at a constant stress rate of $6 \times 10^{-8} \mu \Gamma$ are shown in Fig. 5. Total dislocation displacement of all dislocations grows approximately linearly at the beginning, and tends to grow more slowly and irregularly thereafter. The dislocation displacement still presents a step-shaped response in Fig. 5(a). Throughout the entire simulation time, every dislocation’s average velocity is discrete, showing that the effects of solute atoms on every dislocation are different. The average velocity of a dislocation here is the ratio of the total dislocation displacement to the total number of steps for the selected dislocation.

Here, we chose five dislocations to discuss their motions in detail. Figure 6(a) shows the displacement versus time curves. The mobile dislocation motion shows a step-shaped variation. The plateau corresponds to the pinning state and the elevation corresponds to the unpinning state. This shows that there are one or more pinning and unpinning cycles during dislocation motion. At time $t_1$, the No. 35 dislocation is in motion, while No. 14 is static. The distribution of dislocations and solute atoms at time $t_1$ is shown in Fig. 6(b). We can find that there are some solute atoms gathering below the No. 14 dislocation and no solute atoms gathering around the No. 35 dislocation, as shown in Figs. 6(c) and 6(d). At time $t_2$, the No. 35 dislocation becomes static and there are some solute atoms gathering above it, as shown in Fig. 6(e).

![Fig. 4: Multi-dislocation motion under constant stresses: (a) 0.0003 $\mu$ and 0.003 $\mu$; (b) 0.03 $\mu$]
FIG. 5: Multi-dislocation motion under the constant stress rate: (a) total dislocation displacement; (b) average velocity of each dislocation

FIG. 6: Dislocation motion and distribution of solute atoms: (a) displacement versus time curves of six dislocations; (b) distribution of dislocations and solute atoms at time $t_1$; (c) solute atoms distribution around No. 14 dislocation at time $t_1$; (d) solute atoms distribution around No. 35 dislocation at time $t_1$; (e) solute atoms distribution around No. 35 dislocation at time $t_2$
In the physical material, the dislocations of pinning and unpinning are usually clustered, which lead to the total dislocation displacement demonstrating a step-shaped response. The simulation results are consistent with the theories of DSA. However, due to the technical difficulties, there are no experimental studies to present the DSA processes at the microscopic scale. Therefore, we do not compare the simulation results with the experimental results in this paper.

4. CONCLUSIONS

A two-dimensional, dynamic Monte Carlo model of multiple dislocations and solute atoms has been presented in this paper. The interactions between single or multiple dislocations and solute atoms under different loading conditions were simulated. In the single dislocation simulation under the constant stress rate condition, the dislocation was pinned by solute atoms and was unable to unpin at a low stress rate. At a high stress rate, the dislocation could not be pinned and its motion persisted continuously. Only at an intermediate stress rate did dislocation motion present a step-shaped pinning/unpinning process. In the multi-dislocation simulation under the unstressed condition, solute atoms gathered below positive dislocations and above negative dislocations, which is consistent with the theory of aging. In the multi-dislocation simulation under the constant stress condition, dislocation total displacement increased with increased stress while the pinning effect decreased with increased stress. In the multi-dislocation simulation under the constant stress rate condition, the dislocation displacement/time curves demonstrated a step-shaped behavior. The clustered dislocation pinning and unpinning usually led to a step-shaped response in the total dislocation displacement. The simulation results of the interactions between dislocations and solute atoms present a microscopic view of pinning and unpinning in DSA, which is consistent with the theoretical DSA description. The results have also shown the validity of the model, and established a foundation for further understanding of this mechanism at the microscopic scale.

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