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DYNAMICAL COMPUTER SIMULATION OF THE EVOLUTION OF A ONE-DIMENSIONAL DISLOCATION PILEUP

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Abstract—The dynamical evolution of a one-dimensional dislocation pileup is numerically studied in this paper. By extending particle methods of computational statistical mechanics, criteria for accurate numerical simulation of the pileup evolution are established. A combination of explicit integration of the equations of motion and dislocation freezing after 40 position oscillations gives a maximum error of 5% in the trajectory of the leading dislocation. Explicit integration preserves spatially oscillatory behavior and is shown to give accurate results. The evolution of the dislocation distribution function shows small density wave formation during the compression phase of the pileup.

1. INTRODUCTION

The problem of determining the equilibrium position of dislocations in a pileup configuration has been treated analytically for many years. Eshelby *et al.* [1] developed a general approach describing the equilibrium positions of different dislocation configurations, including the pileup. Their work was based on the work of Stieltjes [2] who treated a similar problem with electrostatic charges. Kanninen and Rosenfeld [3, 4] further developed the work of Eshelby *et al.* [1] to describe the dynamics of dislocation pileup formation. Head [5] and Head and Wood [6] presented a series of papers on dislocation group dynamics and determined the equilibrium distributions of discrete and continuous sets of dislocations. Their work included a derivation of the dynamic evolution of a group of dislocations, and distributions resulting from the formation and release of a dislocation pileup.

Ockendon and Ockendon [7] expanded on the notion of a continuous distribution of dislocations and arrived at a more rigorous description of dynamic dislocation pileups. In more recent work, Balakrishnan *et al.* [8] found an exact solution for the equilibrium dislocation distribution using a continuum model of interacting parallel dislocations moving in a common slip plane.

In all of these theoretical treatments, the equilibrium positions of the dislocations have been accurately determined. The evolution of the dislocation pileup and general movement toward equilibrium positions, however, were only treated with approximate analytical formulations. The study of dynamic dislocation behavior in response to applied forces has not enjoyed enough attention. A mechanistic understanding of time-dependent deformation mechanisms requires a detailed analysis of dynamic dislocation behavior.

The advent of supercomputers has presented alternative ways to study the movement of dislocations within a solid medium. Computational statistical mechanics has been used to examine the individual and collective motion of particles in several types of media; faster computers have allowed the study of increasingly larger numbers of particles. Application of these techniques to dislocation mechanics has only recently been found to be effective in describing, for example, the motion of a dislocation subboundary under the application of stress [9, 10].

In this work we demonstrate the use of computational statistical mechanics, in particular molecular dynamics (MD) theory, to study the evolution of a one-dimensional (1-D) dislocation pileup. In Section 2 we present a general methodology for the solution of the equations of motion. Results are given in Section 3, followed by conclusions of the work in Section 4.

2. NUMERICAL SIMULATION METHODOLOGY

2.1 One-dimensional equations of motion

The 1-D equations of motion for each dislocation is based on fundamental force balance and the interaction between dislocations. Each dislocation represents a point particle which, in a continuum mechanics sense, exhibits a force proportional to $1/r$, where r is the radial distance from the dislocation. Dislocations glide along one crystallographic direction and are not assumed to cross-slip onto adajcent slip planes in a pileup. No dislocation climb is considered in the present model.

For edge dislocations, the position of a group of dislocations placed on line, upon reaching equilibrium, can be determined by solving the following equations:

$$\frac{\partial x_j}{\partial t} = M\sigma^m(x_j), \qquad j = 1, \ldots, n, \tag{1}$$

$$\sigma(x_j) = S(x_j) + A \sum_i \frac{1}{x_j - x_i}, \qquad i = 1, \ldots, n, \tag{2}$$

where

$\sigma(x)$ = total stress,
$S(x)$ = applied stress,
$A = \mu b/2\pi(1-\nu)$,
x_j = position of jth dislocation,
x_i = position of ith dislocation,
M = dislocation mobility.

Solution of this set of equations analytically in a discrete sense is achievable only by letting the stress exponent $m = 1$, and by assuming that the relative positions of the dislocations are constant in time [5]. For $m \neq 1$, the set of equations must be solved numerically and still the solutions only represent an approximation to the exact dynamical behavior of a group of dislocations.

Equation (1) with (2) can be solved exactly, for one dislocation piling up against an obstacle. The solution is given by

$$x = X_{eq}[1 - e^{(S/A)(X - X_0 - V_a t)}] + X_0 e^{(S/A)(X - X_0 - V_a t)}, \tag{3}$$

where

X_0 = initial dislocation position;
$X_{eq} = X' - (A/S)$ = equilibrium dislocation position;
X' = position of obstacle;
S = applied stress (constant value);
V_a = applied velocity = $M \cdot S$.

This solution (3) will be compared to the solution predicted by the simulation in Section 3 [eqn (12)].

Equation (1) in the general discrete form can be rewritten in simpler terms to describe the motion of a dislocation due to individual forces. The general force one dislocation exerts on another is given by

$$\mathbf{F} = (\mathbf{b} \cdot \boldsymbol{\sigma})\mathbf{x}\xi, \tag{4}$$

where ξ is the dislocation line vector, b is the Burgers vector, $\mathbf{F}$ is the net force, and $\boldsymbol{\sigma}$ is the total stress at the dislocation. The velocity is given by

$$\mathbf{V} = \mathbf{V}_a + M\mathbf{F} \tag{5}$$

where M = glide mobility = $D_g b/kT$ and D_g = glide diffusion coefficient.

2.2 Numerical algorithm

2.2.1 Equations of motion. The simulation of dislocation motion consists of applying MD to the equations of motion. In conventional MD, these equations are represented by an explicit central difference formula in molecular positions [11]. Explicit integration methods are more suitable for solving systems of equations for MD. In implicit methods, the savings in computational time by using a larger time step than one for explicit methods is overcompensated by the consumption in time due to the evaluation of the Jacobian for a large number of particles for that timestep [12]. Applied to the dislocation system, the position and velocity are given by the following equations:

$$F_i = F(r_i) = b \sum_{j=1}^{N} \sigma_i(r_j), \tag{6}$$

$$v_i = MF_i, \tag{7}$$

$$r_i = r_{i-1} + v_i \, \Delta t. \tag{8}$$

This system of equations represents a direct application of the particle method [13, 14] in which the numerical algorithm follows the path of the characteristics of the original differential equation. For a large number of particles in the system, errors on the order of Δt are reduced by ergodic mixing [15] which guarantees statistical error cancellation due to the application of the particle method.

2.2.2 Timestep. The value of the timestep in (7) must be chosen for the entire system of dislocations. This timestep must be limited to the minimum amount of time it would take two dislocations to experience a reaction, whether it be collision or annihilation. If we consider two dislocations of arbitrary Burgers vectors coming in close vicinity to one another, the timestep can be expressed by the following condition:

$$\Delta t = \min(\Delta r_{ij}/\Delta v_{ij}), \tag{9}$$

where

$$\Delta r_{ij} = |r_i - r_j|, \tag{10}$$

and

$$\Delta v_{ij} = |v_i - v_j|. \tag{11}$$

In a molecular dynamics simulation (MDS), the balance of forces determines the status of the dislocation position. A dislocation can never reach a true state of equilibrium as long as there are dynamic forces acting on the dislocation. If we treat the 1-D situation of one mobile dislocation piling up against an obstacle as characteristic of a nonequilibrium situation, we can represent the physical picture as a description of the effective potentials of the system.

Figure 1 depicts the potential profile of such a scenario. A locked dislocation is located at the far left. The potentials depicted by the solid lines are due to a single mobile dislocation

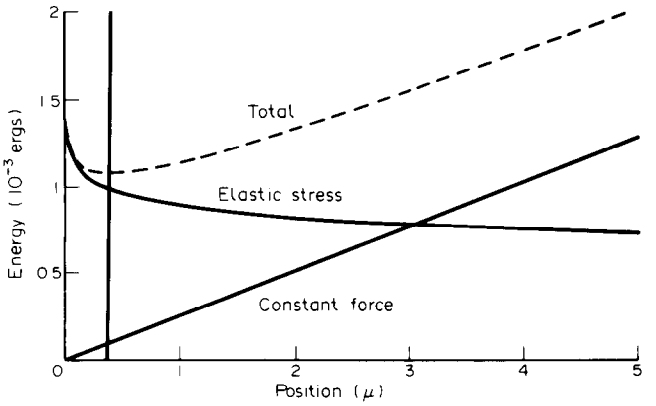

Fig. 1. Potential diagram for single dislocation pileup.

entering from the right toward the obstacle. The vertical line at position $=0.374\mu$ is the equilibrium position of the mobile dislocation for a force $\sigma = 10^8\,\mathrm{dyn/cm^2}$ applied from the right toward the left direction. The solid line of constant slope entering from the right is the potential due to the application of a constant force. The curved solid line at the left starting from infinity and decaying to the right is a logarithmic potential due to a $1/r$ force produced by the locked dislocation. The dotted line is the total of the two potentials.

It can be seen that a mobile dislocation entering from the right will essentially be falling into a potential well. The computer simulation is a finite system, however, and in a finite system this dislocation will never reach an equilibrium position. This matter is complicated by the fact that the potential acting on the dislocation due to the obstacle is greater at the same distance away from the equilibrium position toward the obstacle than the potential on the opposite side. This can be seen in Fig. 1, and it is clear that if an equal timestep is chosen when a dislocation passes through the equilibrium point toward the obstacle, the dislocation will be thrust on the opposite side of the equilibrium point further away from where it started. This problem sets another limitation on the timestep chosen for the calculation. In addition to the timestep being naturally limited by the time it takes two dislocations with the most potential for interaction to interact, the timestep is limited by the approach of one dislocation to the equilibrium position with respect to another.

Figure 2 is a depiction of the trajectories of a mobile dislocation entering from $y = 0.0\,\mu$ toward a locked dislocation at position $y = 1.0\,\mu$. Rotated 90 deg counterclockwise, this figure corresponds to the first $1-\mu$ block of Fig. 1 (the dotted equilibrium line in Fig. 2 corresponding to the solid vertical line in Fig. 1). The scaled time t_0 is the time it would take a dislocation at the origin to arrive at the position of the lock in one timestep. This definition is characterized by eqns (9)–(11).

In the case of a dislocation interacting with a lock, we define the timestep to be a fraction of t_0 (i.e., $\Delta t = f t_0$). The exact trajectory of the mobile dislocation [given in Section 3 by eqn (12)] is represented by the solid line in Fig. 2 curving toward the equilibrium position. The discrete points are applications of the numerical algorithm eqns (6)–(8), and timestep criterion eqns (9)–(11) scaled by various values of f. It can be seen from the trajectories that if the timestep chosen is too large, the dislocation will occupy a position far away from equilibrium on the following timestep and take longer to converge to the equilibrium point. The average relative error is found to be 36% for $f = 1/1.5$, 9% for $f = 1/5$, and 3% for $f = 1/15$.

Choosing a scaling factor $f = 1/5$ appears to be sufficient to accurately represent the trajectory predicted by the analytical solution, but this factor is an unknown in more complicated dislocation configurations. In these cases the equilibrium position is indeterminable analytically, and making the scaling factor arbitrarily small will only serve to escalate computer costs. Therefore, in addition to scaling the timestep by a factor the order of 1/10, an approach to choosing a reasonable timestep based upon methods used in MDS is suggested.

If a dislocation is approaching an obstacle, and at some point changes direction, then a point

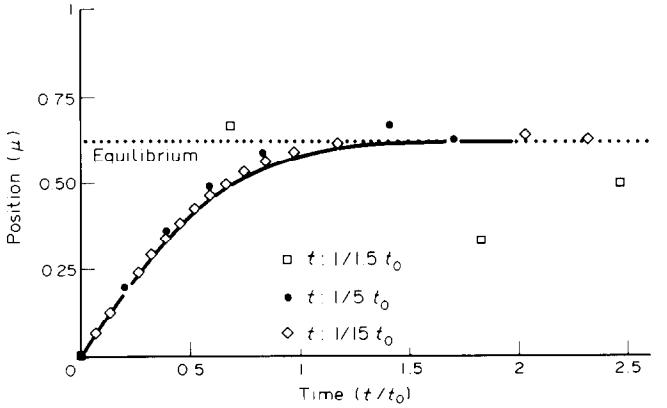

Fig. 2. Dislocation trajectory for single dislocation pileup.

of equilibrium is potentially near. In some MDSs, the change in velocity is used as a detection of an equilibrium point, and the particle is then frozen at its position in place [16]. In simulation of dislocation systems, this change in velocity will be used to limit the dislocation's own velocity in the reverse direction. In other words, it is assumed that the dislocation reversing its velocity will travel no further than the point from which it started in the initial direction before changing velocity. This allows the simulation to proceed without having to rescale the timestep, and also prepares the dislocation to be immobilized if it is indeed close to an equilibrium position.

2.2.3 Dislocation freezing. If the interacting dislocations which determine the timestep are approaching a stable configuration, then the timestep may be permanently determined by those two dislocations for the duration of the simulation. Once dislocations are immobilized however, they are no longer necessary for the determination of the timescale for the simulation. Therefore, these dislocations may be decoupled from the calculation of timestep, but they still participate in the determination of the forces. This technique is termed dislocation freezing in reference to a similar treatment of molecular systems in which particles come close to equilibrium positions.

Figure 3 shows the evolution of the trajectories of the first 7 dislocations from a simulation of a 50-dislocation pileup. This particular calculation was performed with a timestep limited to the time it would take the dislocation with the largest force to react with another dislocation, or obstacle, using a scaling factor of $f = 1/10$. For the entire simulation, that dislocation is represented by the leading dislocation in the 50-dislocation pileup. It is seen in Fig. 3, however, that this dislocation reaches equilibrium early in the simulation. In fact, it is in an equilibrium position and, for all practical purposes, it is an immobile dislocation.

It is therefore not necessary to include this dislocation in the computation of the global timestep, and so it would be practical to remove this dislocation from the reaction calculation. The difficulty with this, in a general sense, is that there is no way to predict the equilibrium position analytically for a pileup of more than one dislocation [5]. In a realistic situation, the dislocations which are in the pileup in equilibrium are in fixed positions, because the force acting on any one of the dislocations is not sufficient to cause an atom from a lattice site to jump to the adjacent lattice position.

In the previous section, it was suggested that a dislocation close to equilibrium be limited in its velocity in the reverse direction. As seen in Fig. 3, the dislocation closest to the obstacle oscillates about the equilibrium point, mostly at the beginning of the simulation but also throughout the time evolution of the simulation. When this dislocation first begins oscillating, it is not quite at equilibrium because the other dislocations in the pileup are continually moving in. It is found that after about 30–40 oscillations, this dislocation eventually reaches equilibrium. The average error produced by the deviation of this leading dislocation from the true trajectory is less than 5%. For the remaining dislocations, it can be seen that the errors are even less than that for the first dislocation. In fact, after about the third dislocation, the

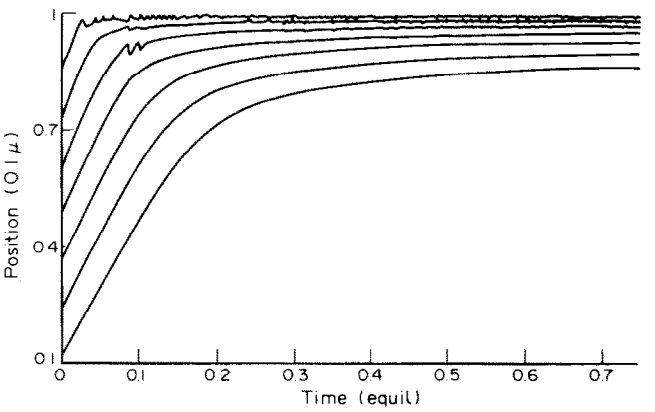

Fig. 3. Free position trajectories for first 7 of a 50-dislocation pileup.

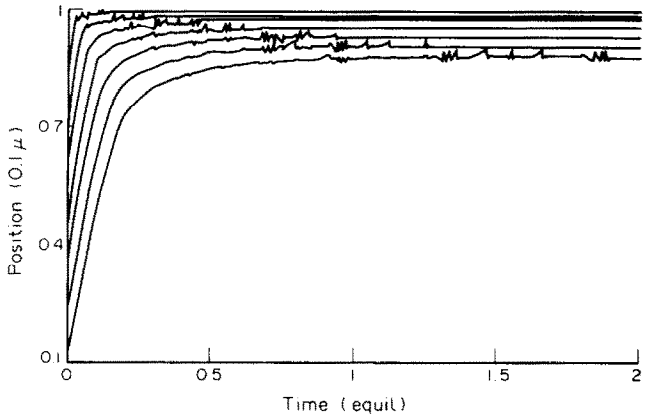

Fig. 4. Freezing position trajectories for first 7 of a 50-dislocation pileup.

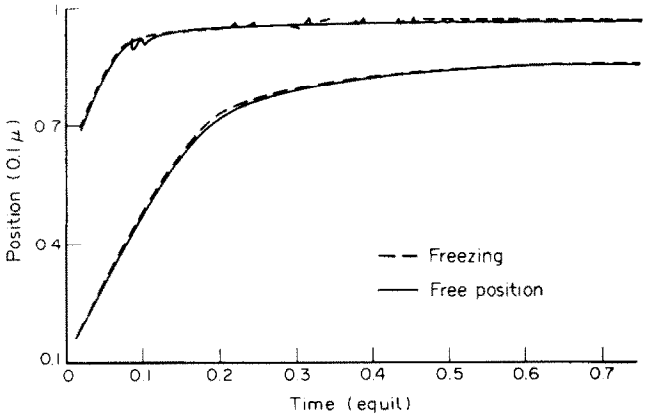

Fig. 5. Comparison of freezing and free position trajectories for 3rd and 7th dislocations of a 50-dislocation pileup.

trajectories are all smooth and there are no significant deviations in the dislocation motion. Therefore the error introduced into the system by assuming a fraction f of $t_0 = 1/10$ is small enough to accurately reproduce the trajectories in a 50-dislocation pileup.

Starting from the dislocations nearest the obstacle, each dislocation is successively monitored for oscillatory motion. After about 40 oscillations from first detection a change in velocity, the position of the dislocation being observed is fixed, and the monitoring process continues for the next dislocation outward from the obstacle. The result of this procedure can be seen in Fig. 4 which shows the trajectories of the first 7 dislocations of a 50-dislocation pileup. A comparison of this freezing technique with the standard evaluation of trajectories in Fig. 5 indicates that the trajectories are identical for both methods. Considering CPU time, it is found that dislocation freezing results in an order of magnitude savings in computer time compared to direct calculations.

3. RESULTS

3.1 Single dislocation pileup

Equation (3) rewritten in terms of the time variable to compare the analytical formulation with the simulation eqns (6)–(8) yields:

$$t = -\left(\frac{S}{AV_a}\right) \cdot \ln\left[\frac{X - X_{eq}}{X_0 - X_{eq}} \cdot e^{-[(S/A)(X - X_0)]}\right]. \tag{12}$$

As previously discussed, Fig. 2 shows that if the timestep chosen is small enough, the simulated dislocation will follow precisely the trajectory predicted by analytical solution to the equation of motion.

3.2 Multiple dislocation motion

Head postulated that a number of dislocations placed at the origin would follow an evolution in time based on the principle that the relative positions of the dislocations would be approximately constant in time [5]. Solutions of this nature to eqn (1) are therefore referred to as similarity solutions, in which the dislocation position can be represented by the following approximation:

$$x_j = X_j g(t). \tag{13}$$

The solution to (1) with this substitution yields, for $m = 1$, a time dependence of the form

$$g(t) = (2t)^{1/2}. \tag{14}$$

Figure 6 represents the evolution of the positions of six dislocations with a lock at the origin when all six are placed at equal spacings at time $t = 0$. It can be seen in this figure that the dislocations follow parabolic trajectories, as predicted by (14). The relative positions of the dislocations reach an equilibrium at t of the order of 3.3×10^6 s, and this is characterized by $t = 1$ in Figs 6 and 7. The latter figure represents the change in relative positions of the dislocations up to the equilibrium spacing as predicted by Head. After equilibrium is achieved, the dislocations remain at this spacing for all time.

3.3 Dislocation distribution evolution

Eshelby *et al.* [1], and others [2–6] have determined the equilibrium positions of individual dislocations which are piled up against an obstacle. For a small number of dislocations, the application of a discrete model such as that proposed by Head provides a computationally feasible method for determining equilibrium positions. For a pileup of a large number of dislocations however, it is suggested [17] that characterization of a continuous distribution of dislocations is as good an approximation as the discrete model. A single pileup of dislocations against an obstacle by a shear stress σ can thus be represented by the following distribution equation [17]:

$$f(x) = \frac{2(1-\nu)\sigma}{\mu b}\left(\frac{L-x}{x}\right)^{1/2}$$
$$= \text{probability per unit length of finding a dislocation at position } x, \tag{15}$$

and the number of dislocations in a particular region (Δx) along the pileup can be calculated in

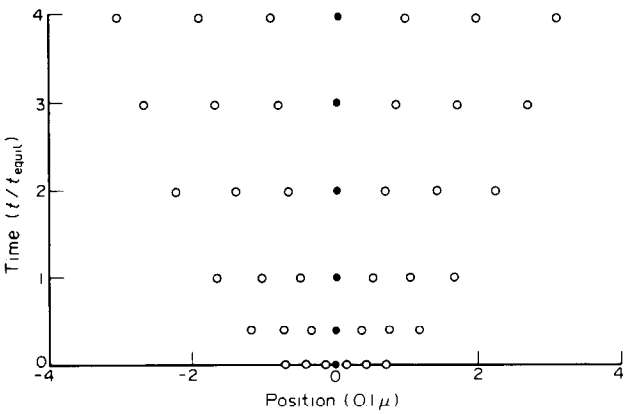

Fig. 6. Dynamic motion of a 6-dislocation expansion with a lock at the origin.

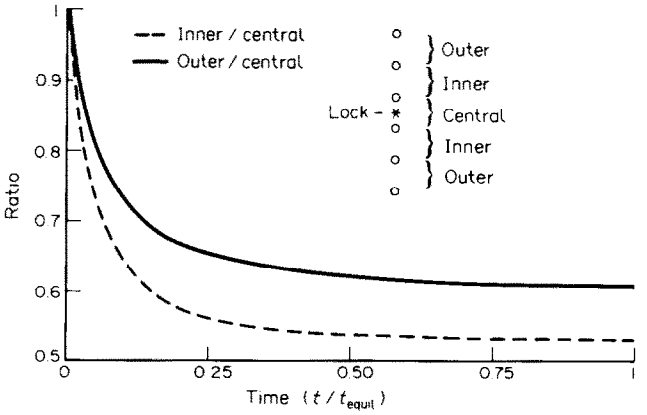

Fig. 7. Dislocation spacing ratios in a 6-dislocation expansion with a lock at the origin.

the following manner:

$$\text{No. of dislocations} = f[x + (\Delta x/2)]\,\Delta x. \tag{16}$$

In comparison with a simulation of dislocation motion, it is useful to know the length of the pileup, determined by the equation

$$L = \frac{\mu N b}{\mu(1-\nu)\sigma}, \tag{17}$$

where L = pileup length and N = number of dislocations in the pileup.

Simulation of a group of a large number of dislocations would produce a distribution of dislocations in which the density of dislocations decreases further away from the obstacle against which the dislocations are piling up. It is found in experiments [18] that a pileup of no more than 50–100 dislocations actually occurs in one dimension. Comparisons were therefore made between the distribution produced by a simulated 50-dislocation pileup and the equilibrium distribution predicted by (15).

If the dislocations are placed uniformly on a line of length a little less than L given by (17), then if a stress is applied in the direction of the dislocation toward an obstacle, the group of dislocations will undergo a dynamic compression. This is shown in Fig. 8 for 50 dislocations. As time proceeds, the pileup shows a progressive concentration of dislocations toward the obstacle, as is expected from the physics. The dynamic behavior of a $1-D$ pileup is similar to the behavior of compressible fluids. Local velocity variations are manifested in dislocation density variations in a manner similar to compressible fluids described by Euler's eqn [19]. Figure 9 shows a comparison of the stages of the evolution of the dislocation pileup, as shown

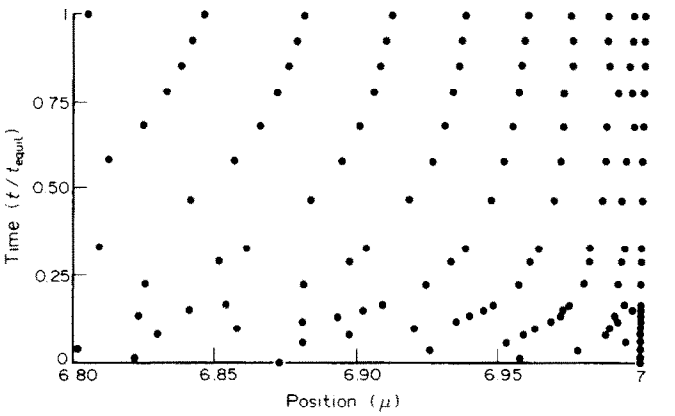

Fig. 8. Dynamic motion of the first few dislocations of a 50-dislocation pileup.

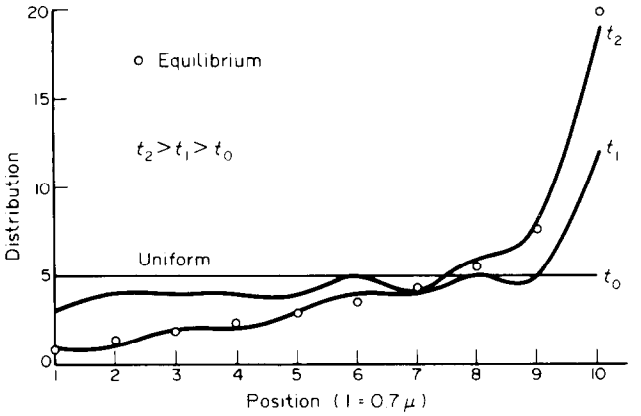

Fig. 9. Evolution of dislocation distribution in a 50-dislocation pileup.

in Fig. 8, in distribution form. The disturbance density waves are eventually dampened when the distribution approaches its equilibrium value, as Fig. 9 shows. It can be seen that the equilibrium distribution generated by the simulation closely predicts the distribution calculated by (15) for 50 dislocations.

4. CONCLUSIONS

It has been shown that methods of computational statistical mechanics can be used successfully to model dislocation dynamics. In particular, the phenomenon of a 1 – D dislocation pileup has been studied. The physics of motion of dislocations in a pileup is found to be similar to the behavior of the motion of a fluid in a dynamic compression. The trajectories of the dislocations during pileup illustrate this phenomenon of compression, in which a fluid pushed in one direction up against an obstacle exerts a back stress in the reverse direction which causes a variation in local fluid density. It is found, however, that the dynamics which represent an accurate simulation of the trajectories are sensitive to the choice of timestep in an explicit difference numerical solution method.

The importance of this choice of timestep is evidenced by the results of the 1 – D simulation for various dislocation configurations. For the case of one dislocation pushed up against a lock, it was found that the timestep criterion dictated by the time to dislocation-dislocation interaction is insufficient to accurately characterize the true trajectory of dislocation motion. Instead, a scaling factor, f, was introduced to reduce the timestep to allow the dislocation to approach the equilibrium position determined analytically by the balance of forces on the mobile dislocation with respect to the lock. This factor was determined to be of the order of 1/10 for an accurate simulation.

In extending the simulation to the motion of a group of dislocations, the deviations from the true trajectories of dislocations in a 50-dislocation pileup produced by using a scaling factor of 1/10 were found to be significantly less than 5%. This error is only characteristic of the dislocation closest to the obstacle, and the error in simulating the trajectories of the remaining dislocations is less than this value. The sacrifice in the exact reproduction of the trajectory of the first dislocation is justified by the savings in computational time which results from assuming a value of the scaling factor, f, which is not too small.

It is found that the equilibrium configuration of an arbitrary collection of dislocations cannot be determined a priori by analytical techniques. Numerical solution of equiibrium positions is possible, but under realistic dynamical conditions, it is difficult to predict which set of dislocations constitutes a group in an arbitrary configuration. Therefore it is suggested that, in addition to scaling the global timestep by a constant factor of the order of 10, a numerical algorithm which detects the approach to equilibrium by monitoring changes in dislocation velocity be applied to the solution procedure.

The results of this technique indicate that if a dislocation within a pileup undergoes more

than 40 oscillations about an equilibrium point with a timestep chosen as previously suggested, the dislocation has essentially attained an equilibrium position. Freezing the dislocation at this point provides a savings in computational time of the order of 1 magnitude of CPU time on a Cray-1 computer, while preserving the accuracy in the determination of the dislocation trajectory.

The results of these 1-D simulations show that the savings in computational time is significant, without sacrificing the accuracy of dislocation trajectories, when the timestep criteria as outlined in this paper is applied. Further implications of these results are that in the extension to two dimensions, similar timestep criteria can be successfully applied, especially in the case of dislocation cell formation. In this event, the number of dislocations which constitute a cell wall is of the order of that which is studied in this paper. The simulation criteria established in this paper will be helpful in the dynamical simulation of 2-D pattern formation for a large number of dislocations (~10,000).

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