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COMPUTER SIMULATION OF DISLOCATION GLIDE THROUGH FIELDS OF POINT OBSTACLES

by

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ABSTRACT

The problem of dislocation glide through microstructure has been simulated in a model in which the dislocation is assumed to be a string of constant tension and the microstructural barriers to glide are taken to be immobile point barriers of given properties. The construction of an efficient and versatile simulation code capable of handling the complex but interesting variants of this problem in reasonable computing time requires the use of sophisticated coding procedures. Central problems include: [1] storing the microstructure, i.e., the location and properties of obstacles, in easily retrievable form; [2] representing the dislocation configurations so that complete information is easily accessible and modifications in the configuration are easily made; [3] constructing an efficient computer algorithm for advancing dislocations according to pre-selected criteria without loss of information. The solutions to these problems are described and the capabilities of the code discussed.

INTRODUCTION

The plastic deformation of a crystal is typically accomplished by the glide motion of dislocations. The glide is driven by the applied stress and opposed by microstructural features such as solute atoms, other dislocations, and precipitates or inclusions. Given the geometric complexity of the dislocation structure and the microstructure in the usual realistic case the treatment of dislocation glide rapidly becomes analytically intractable, even when rather simple assumptions are made about the properties of the dislocations, the obstacles, and their interactions. In analytic treatment of dislocation motion one is usually forced into idealizing assumptions concerning both the critical events which govern glide and the manner in which these events sum statistically to yield glide conditions or glide rates.

The availability of large computers adds a new dimension to the study of dislocation motion. Since these are capable of rapid numerical calculation, of storing and recalling complex geometrical information, and of modelling simultaneous interacting processes the efficient use of computers allows the study of dislocation models in much more elaborate detail. While computer models, like any theoretical models, require initial idealizing assumptions the number of these assumptions may be greatly reduced and the richness of the results significantly enhanced.

Our own computer simulation research has concentrated on the effects of the configuration of dislocations and the nature and distribution of microstructural barriers on the critical shear stress and on the velocity of thermally activated glide. Given the intent of this work the properties of the dislocations and the microstructural barriers have been modelled in the simplest plausible way so that the full power of the computer could be devoted to providing the geometrical structure needed to give good statistical detail.

In the basic problem studied here (1) the dislocation is modelled as a flexible, extensible line of constant tension, Γ, and Burgers vector of magnitude b. The dislocation is assumed to glide in a plane containing a known (usually Poisson) distribution of point barriers (2) of given properties, whose density is characterized by the mean area (a) per point or by the characteristic length $\ell_s = (a)^{1/2}$. A dislocation segment pinned by two such obstacles under a resolved shear stress, τ, in the glide plane is bowed out into a circular area of radius

$$R = \Gamma/(\tau b) \tag{1}$$

or, in dimensionless form,

$$R^* = R/\ell_s = \Gamma/(\tau \ell_s b) \quad . \tag{2}$$

It is possible and convenient to express the shear stress in a dimensionless form, τ^*, which simplifies its relation to the bow-out radius, R^*:

$$\tau^* = 1/2R^* = \tau \ell_s b/2\Gamma \quad . \tag{3}$$

The interaction between the dislocation and a point barrier is illustrated in Fig. 1. The force exerted on the obstacle can be calculated (2) by resolving the line tension of the two neighboring dislocation arms:

$$F = 2\Gamma \cos(\psi/2) \qquad (4)$$

where ψ is the included angle between the dislocation arms. This force may be conveniently made dimensionless:

$$\beta = F/2\Gamma = \cos(\psi/2) \quad . \qquad (5)$$

If F_c is the critical value of the force at which the dislocation will bypass the obstacle, the strength of the obstacle may be denoted by the corresponding dimensionless force β_c ($0 \leq \beta_c \leq 1$). If the dislocation is allowed to bypass the obstacle through thermal activation then a more detailed specification of the dislocation-obstacle interaction must be given. It is sufficient to specify the function $G(\beta)$ giving the activation barrier to glide as a function of the applied force.

A solution to the problem of plastic deformation in the simple model outlined above should predict at least three types of information: [1] the athermal yield stress, or critical resolved shear stress for athermal glide (τ_c^*), which depends upon the distribution of dislocations, the nature of dislocation interactions, and the strength and distribution of the barriers; [2] the rate of deformation, which depends additionally on the applied stress, the temperature (which may also be set in dimensionless form (1)) and the specific nature of the dislocation-obstacle interaction (i.e., on $G(\beta)$); [3] salient morphological features of the deformation process, including in particular the temporal ("jerkiness") and spatial heterogeneity of flow. The solution should, moreover, be phrased in analytic form, either as the analytic solution to a well-posed subproblem or as an accurate analytic fit to probative computer-generated data.

Given these desirable features a suitable computer simulation code should have at least the following capabilities: [1] the flexibility to simulate a variety of interesting cases; [2] the ability to generate accurate data on the critical resolved shear stress and the flow rate for non-trivial models in reasonable computer time; [3] the ability to monitor the deformation process in sufficient detail that critical mechanistic features may be identified and isolated for detailed study; [4] the capability of computing and retrieving the specific data needed to assess and criticize theoretical models. A code which generally satisfies these criteria has been in use at Berkeley for some time. In the following section the central features of that code are described. The concluding section briefly lists some of the problems to which it has been addressed.

BASIC CODING TECHNIQUES

In the basic problem simulated in this research a dislocation (or set of dislocations) is introduced into a glide plane (or set of glide planes) containing a distribution of point barriers of specified properties. A stress is applied and the dislocations are allowed to move freely until they find themselves in obstacle configurations which cannot be passed mechanically under the applied load (adjusted for dislocation interactions).

Subsequent behavior depends on the process being simulated. In simulating athermal glide the applied stress is increased until the dislocation configuration just becomes mechanically unstable. The dislocations are then displaced through the array until a new stable configuration is found. This process of raising the stress to the minimum point of instability and advancing the dislocations until a new stable configuration is found is continued until a value of the stress is reached at which no further stable configurations occur. The lowest such value is the critical resolved shear stress, τ_c^*. The salient feature of the athermal glide process is the strength-determining configuration, the configuration of dislocations and obstacles which is most stable mechanically, and hence determines τ_c^*.

In simulating thermally activated glide the applied stress is held constant and the activation barrier computed at each pinning point in the configuration. The site for thermal activation is then chosen using proper statistical procedures (1) (or well-defined approximations to them). The activated site is broken, and the dislocations advanced until a new stable configuration is found. This process is iterated and the velocity of glide computed from statistical formulae (1). The salient features of thermally activated glide is the sequence of stable configurations encountered during passage through the obstacle array; the geometric properties of these configurations determine the relevant activation barriers.

The precise code used to simulate the processes described above depends on the specific case under study, e.g., whether we are treating an isolated dislocation or several dislocations which interact with one another, whether the obstacles are assumed to be athermal or thermally activated. These various specific codes are, however, obtained by varying the peripheral features of a code which depends upon three central techniques: [1] a method for storing obstacle arrays so that local subsets can be easily accessed; [2] a data structure for dislocations which carries all relevant information in a compact form and allows efficient modification as the dislocation is moved; [3] a consistent algorithm which advances dislocations efficiently and without loss of information.

1. Storing the Obstacle Array

Clearly any algorithm for locally advancing a dislocation need consider only the obstacles in the immediate vicinity of the portion of the dislocation currently being advanced. It is hence efficient to store the obstacle array in subarrays such that only the relevant local subarrays need to be accessed and considered when locally advancing the dislocation. If a subarray has an area, A, containing randomly distributed points of density one then the probability, $\rho(n,A)$, of finding n points in the subarray is

$$\rho(n,A) = \frac{A^n}{n!} \exp(-A) \quad . \tag{6}$$

Inverting this function, a random number generator can be used to determine the number of points in each subarray. Thus by choosing the dimensions of the subarrays each subarray can be constructed individually.

The subarrays may be filled in one of two ways. If the total size of the array is relatively small so that computer storage is not an issue one may simply fill the subarrays by using a random number generator to establish the x and y coordinates of the points contained. The x and y coordinates of all points may be stored in ordered one-dimensional arrays with additional ordered one-dimensional arrays, as needed, containing the strengths and other pertinent properties of the individual obstacles. Two additional arrays of dimension two are used to store the start and end location of each subarray in the x and y arrays. Thus a directory is created for finding the necessary local subregions of the entire array. The directory also allows efficient storage of the x and y arrays. Finally, each obstacle is marked with a digit indicating whether it is behind, ahead of, or on a given dislocation.

When the simulation considers either glide through large arrays or simultaneous glide in several arrays computer storage becomes relevant. A straight-forward and useful alternative method may then be used. Rather than storing the entire array the seeds for the random number generator for each subarray are stored in the directory on construction of the subarrays previously described. Then no subarray need be retained in storage since each can be constructed consistently as needed. Arrays can be recorded and reproduced in separate experiments by simply recalling (or consistently regenerating) the subarray structure and the associated seeds.

If the subsequent reproducibility of the particular obstacle array is not necessary to the simulation experiment an even more efficient technique may be used. The only a priori information known about a random array of obstacles is its density, which is, in this problem, identically one if the unit of length is taken to be ℓ_s. It is hence statistically permissable to construct random subregions as they are needed when the dislocation is advanced. Since the dislocation does not know what is in front of it, and does not remember what is behind it, the only obstacle information which ever need be actively in storage is the nature and location of the obstacles which are actually in contact with the dislocation and the nature and location of the obstacles immediately in front of the specific local section of the dislocation which is currently being advanced. In this way the glide of an isolated dislocation through an array of very large size may be efficiently treated with minimal demand on computer memory.

These are the basic algorithms used in the simulation code to efficiently create, store, and retrieve the obstacle arrays. The modification of these techniques to treat non-random distribution is straight-forward.

2. Representing the Dislocation

To optimize the information obtained from the simulation of glide it is important that the dislocation (or dislocations) be stored in the computer in a simple array which contains all relevant information and can be easily accessed and updated. These criteria are efficiently met by a data structure in which a dislocation is represented by a two-way chained list. The central element of this structure is a simple ordered list of the x and y coordinates of the obstacles in current contact with the dislocation. Each obstacle in this list is then connected to two identifiers which give the location in storage of the obstacles to its immediate left and right, and to a mark which indicates whether the mechanical stability of the dislocation segment to the right of the obstacle has been verified. The configurations of several dislocations may be simultaneously stored by adding a list of pointers to one obstacle on each dislocation; given periodic boundary conditions the sublist representing a single dislocation will be closed under the operation of left and right connection.

All relevent information concerning the dislocation, such as the shapes of inter-obstacle segments, the forces on the obstacles, and the mechanical stability of the configuration, may be easily computed from the information contained in this double-chained list. When the dislocation is advanced the by-passing of an obstacle is accounted for by simply deleting it from the list and updating the relevant connections; contact with a new obstacle is achieved by simply adding it to the list. Interesting configurations, such as the strength determining configuration may be stored for later study by simply copying the list in storage.

3. Advancing the Dislocation

The dislocation is advanced in the code by the analytic equivalent of the following procedure. A dislocation configuration becomes unstable by bypassing an obstacle along it, either because of mechanical instability of the segment to the left or right of the obstacle due to increasing stress or because the obstacle has been passed by thermal activation according to some criterion. This obstacle is appropriately marked and removed from the list representing the dislocation, the obstacles to its left and right are connected in the list and the associated segment is marked to indicate that its stability has not been verified.

The new dislocation segment will bow out between its terminal obstacles toward equilibrium. This bow-out process will be terminated by the first of three events: [1] the dislocation encounters a new obstacle of the array; [2] the dislocation violates the angle condition $\psi > \psi_c => \beta < \beta_c$ at one of its two end points; [3] the dislocation segment bows into the equilibrium radius $R^*(= 1/2\ \tau^*)$. To determine the first of these events we utilize a geometric relation (Fig. 2): if a circular arc is drawn through two points A and B, and if a third point, C, is located on this arc and connected to A and B by lines $\overline{AC}$

and $\overline{CB}$, then the angle, α, measured clockwise between the extension of $\overline{AC}$ and $\overline{CB}$ is given by

$$\alpha = \sin^{-1} (\overline{AB}/2R) \tag{7}$$

where $\overline{AB}$ is the distance from A to B and R is the radius of the arc. Using the terminal conditions [2] and [3] a maximum value, α_m, may be found at which the bow-out process necessarily terminates. The area of the array associated with bow-out to α_m may then be identified and the values of α_i computed for each obstacle, C_i, within this area.

If there are obstacles having $\alpha_i \leq \alpha_m$ then the particular obstacle having the minimum value of α would be the first contacted by the dislocation in a continuous bow-out process. The obstacle is added to the dislocation and the list is updated to correct for its connections to left and right. The corresponding sections are marked and their stability or possible further subdivision is tested in turn.

If there are no obstacles having $\alpha_i \leq \alpha_m$ then the appropriate terminal condition [2] or [3] is invoked. If condition [2] pertains then the unstable end point is by-passed by properly marking it, removing it from the list, and updating the list. The update defines a new segment whose stability must be tested. If condition [3] pertains then a stable segment has been found. When the list representing the dislocation contains only stable segments a stable configuration has been found.

When the dimensionless applied stress is high ($\tau^* \gtrsim 0.5$) an additional check must be made for possible instability due to self-intersections of the dislocation and a procedure must be provided to decompose the dislocation list to account for the formation of stable loops from self-intersections during glide. The procedures for handling these cases are straight-forward using the data structure and search algorithm described. At lower values of τ^* such intersections are extremely uncommon, and may usually be ignored.

A stable configuration may be broken by either increasing the stress or selecting an obstacle for thermal activation. The stress at which the configuration first becomes unstable may be precisely calculated, and corrected for possible contact with additional obstacles during bow-out as the stress is raised. The athermal critical resolved shear stress is that value of τ^* which is just sufficient to insure that no stable configurations are found. It may be found by continuously increasing τ^* until no further stable configurations are encountered.

This data structure and search algorithm combine to yield a code whose efficiency is sufficient for our own research purposes. In current use on the CDC 6600/7600 system at the Lawrence Berkeley Laboratory the code requires $\sim$25 computer units ($\sim$8 seconds) of running time to determine the athermal resolved shear stress for glide through an array of 10^4 points together with a geometric analysis and TV-graphic plot of the strength determining configuration. The simulation of thermally-activated glide is only slightly less rapid. The simulation of glide through very large arrays is relatively time-consuming, but not prohibitively so. Analysis of glide through a square array of 10^6 points requires $\sim$1500 computing units ($\sim$7-1/2 minutes).

APPLICATION

The coding procedures described above have been used to conduct simulation studies on a variety of problems in dislocation glide. Many of the central results of these studies have, or shortly will be, published elsewhere. Research to date includes the following.

1. Glide of a single dislocation through an array of like obstacles

The athermal critical resolved shear stress for glide through a random array of like obstacles was previously investigated by Kocks (3) (for the particular case of impenetrable obstacles) and by Foreman and Makin (4). In the present program these studies were extended to include the statistics of the athermal glide stress and the detailed features of the particular obstacle configurations which determine the glide stress (5). Based on the insight provided by these studies analytic equations were developed to estimate the athermal glide stress and the geometric properties of the strength-determining configurations which determine the glide stress (5). Based on the insight provided by these studies analytic equations were developed to estimate the athermal glide stress and the geometric properties of the strength-determining configurations in the limit of large array size (6). To test the validity of these equations it was necessary to simulate glide through very large arrays (7). Fig. 3 is taken from this work, and presents the athermal critical resolved shear stress as a function of array size for square arrays of up to 10^6 obstacles of strength β_c = 0.01.

The thermally activated glide of a dislocation through a random distribution of point barriers was investigated in mechanistic detail (5). In earlier theoretical work (1) the statistics of thermally activated glide were developed and useful approximations identified. These approximations were studied through simulation and their range of accuracy identified (5,8). The work was extended (8) to investigate the rate and morphology of the thermally activated deformation of an idealized crystal deforming through the planar glide of non-interacting dislocations.

2. Glide through fields of unlike barriers.

The analytic procedure developed in reference (6) to estimate the critical resolved shear stress for glide through an array of like barriers was extended to treat the case of simultaneous random distributions of obstacles of different properties (9). The predictions of the equations were compared to the results of simulation experiments on glide through arrays containing both strong and weak obstacles. Relevant properties of the strength-determining configurations were determined, including the distribution of angles and segment lengths and the relative fractions of strong and weak obstacles. More recent work (7) has included simulations of thermally activated glide through mixed arrays of strong and weak obstacles, studies of the athermal glide stress in arrays containing distributions of obstacle properties, and large array simulations probing the initial effect of a small admixture of relatively strong obstacles on glide through an array of relatively weak obstacles.

3. Simultaneous glide of interacting dislocations.

The coding procedures described here can be directly used to simulate the simultaneous glide of interacting dislocations so long as the internal stress due to dislocation interaction can be reasonably approximated as constant over each dislocation segment. Recently the code has been used to simulate the glide of both planar and vertical arrays (low angle grain boundaries) of like dislocations (7). Athermal glide stresses have been determined as a function of dislocation density (grain boundary angle) in both these cases and the strength-determining configurations have been identified and studied. Examples are presented in Fig. 4. The simulation of the evolution of distributions of unlike dislocations distributed over parallel glide planes is within our capability, and will be done in the near future.

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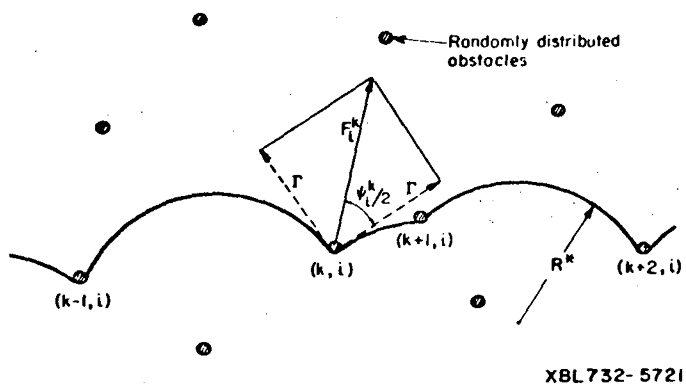
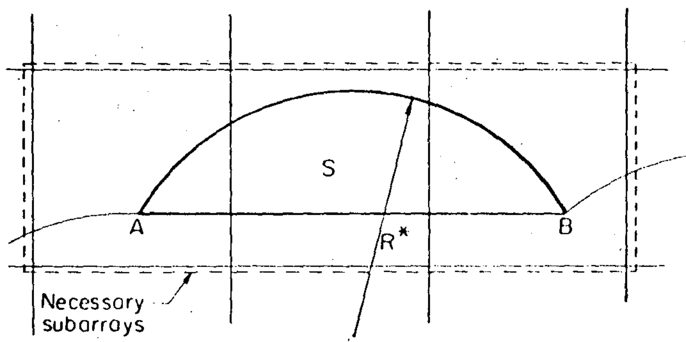
FIG. 1



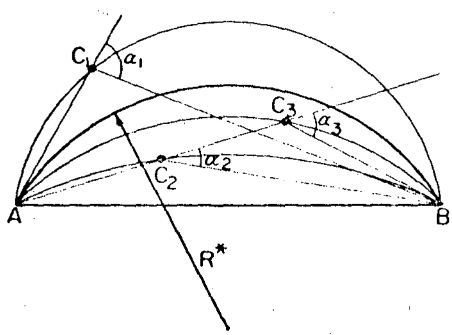
Equilibrium of a dislocation under stress.

FIG. 2

PARAMETERS FOR DISLOCATION MOTION ALGORITHM



(a)



(b)

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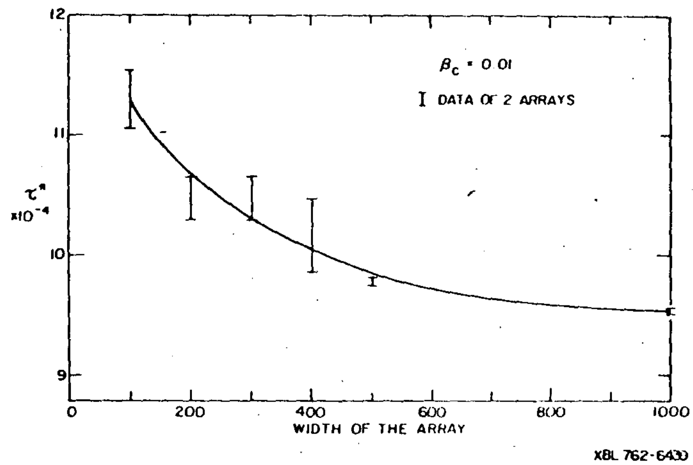
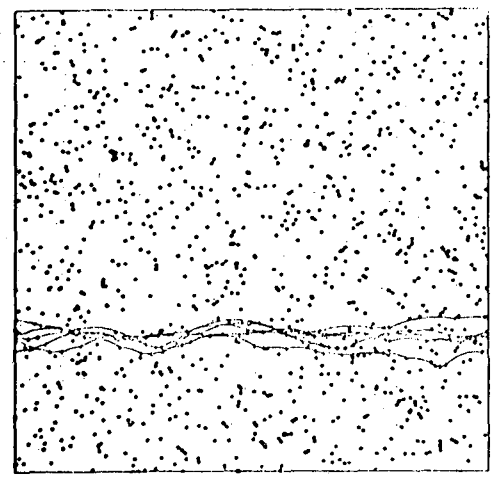
FIG. 3



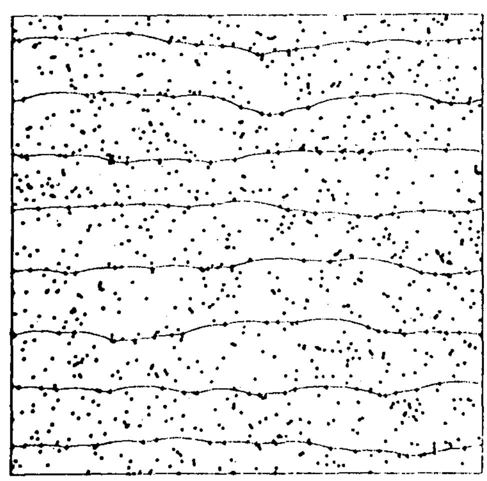
The variation of the athermal glide stress with array size for glide through a random array of obstacles of strength β_c = 0.01.

FIG. 4

EXAMPLES OF INTERACTING DISLOCATIONS



(a) 5 Parallel glide planes



(b) 8 Dislocations in series

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