Submitted to Journal of
Applied Physics

LBL-1166
Preprint c.1

THERMALLY ACTIVATED GLIDE THROUGH A RANDOM ARRAY OF OBSTACLES: I. STATISTICS OF THERMAL ACTIVATION

J. W. Morris, Jr. and Dale H. Klahn

March 1973

Prepared for the U.S. Atomic Energy Commission
under Contract W-7405-ENG-48

THERMALLY ACTIVATED GLIDE THROUGH A RANDOM ARRAY OF OBSTACLES: I. STATISTICS OF THERMAL ACTIVATION

J. W. Morris, Jr. and Dale H. Klahn
Department of Materials Science and Engineering
University of California, Berkeley and
Inorganic Materials Research Division,
Lawrence Berkeley Laboratory

ABSTRACT

This paper treats the statistics of thermally activated glide of a dislocation, modelled as a string of constant tension, through an array of randomly distributed, identical, immobile point obstacles. The parameters governing thermally activated glide are defined and equations are developed giving the expected value and variance of the time to activate through an obstacle array or sequence of arrays in terms of the properties of the obstacle configurations encountered. The proper statistical definition of the velocity of glide is discussed. It is shown that the velocity of glide, as determined from the strain rate, is simply proportional to the inverse of the expected time to transit the array (or sequence of arrays). Simplifying approximations are identified for use at low temperature or high stress. We finally discuss how these statistically relations and approximations may best be used in numerical simulation of thermally activated glide.

I. INTRODUCTION

The mechanical behavior of a crystalline solid is often influenced by dislocation motion through a field of obstacles, for example, forest dislocations, solute atoms, or small precipitates, which are dispersed in a more or less random fashion through the crystal. The problem of predicting the rate of this dislocation motion is formidable. We have been engaged in a study of one of the simplest problems of this type: the thermally activated glide of a dislocation, idealized as a line of constant tension, through a random array of identical, immobile point obstacles under constant applied stress.

The problem may be described as follows (Figure 1). Consider a crystal plane which is the glide plane of a dislocation. Let it contain a random distribution of points which act as obstacles to dislocation glide. Let an initially straight dislocation be introduced at one edge of the plane, and let this dislocation glide into the plane under the action of a resolved shear stress. The dislocation glides freely across the empty initial area of the plane. It may also mechanically pass some of the point obstacles, either by cutting through them or folding around them to close on itself. This glide continues until the dislocation finds itself in a configuration in which it is pinned along its whole length by obstacles which it cannot pass mechanically. Such a configuration is illustrated in figure 1. If the dislocation is confined to the glide plane and the stress is held constant the dislocation remains pinned in this stable configuration until thermal activation carries it past at least one of the pinning obstacles. It then glides until a second mechanically stable configuration is reached and the process of thermal activation must be repeated. The problem is to compute the expected value of the velocity of dislocation glide through repeated thermal activation as a function of the applied stress, the temperature, and the nature and density of the point obstacles.

The solution of this problem requires two types of information. First, we need to know the relevant properties of the mechanically stable configurations assumed by the dislocation as it glides through the obstacle field. Second, we need the proper statistics of thermally activated glide through these configurations. The present paper is principally devoted to the second part of the problem. In the following sections we identify our assumptions and write the governing equations of simple glide through a random array of point obstacles at finite temperature, then develope the statistics of thermal activation.

To obtain the distribution of line strengths we employ a computer code which numerically simulates thermally activated dislocation glide. The code, its use, and initial results will be discussed in the second paper[1] of this series.

II. ASSUMPTIONS AND BASIC EQUATIONS

Let a random array of points fill a square segment of a plane. The array is described by the statement that its points are randomly distributed and by a characteristic length

$$l_s = (a)^{1/2}, \tag{1}$$

where a is the average area per point. The total area of the square segment is

$$A = n\,(l_s)^2, \tag{2}$$

where n is the total number of points contained. In dimensionless form, the area is

$$A^* = {}^{A}/(l_s)^2 = n \tag{3}$$

and the dimensionless edge length of the square segment is

$$L^* = n^{1/2}. \tag{4}$$

Let a dislocation be introduced into the square segment. The dislocation will be treated as a flexible, extensible string characterized by a line tension (Γ), its energy per unit length, and by a Burgers vector ($\underset{\sim}{b}$), of magnitude b. The line tension is assumed constant; we neglect any dependence of Γ on the orientation of the line or on the mutual interaction of segments of the line. The Burgers vector is taken to lie in the plane.

Let a stress $\underset{\sim}{t}$ be applied to the body containing this plane. If the dislocation moves so as to sweep out area A under the action of this stress the work done is [2]

$$\delta W = \tau b \delta A \tag{5}$$

where τ is the resolved shear stress

$$\tau = (\underset{\sim}{b} \cdot \underset{\sim}{t} \cdot \underset{\sim}{n})\, b^{-1} \tag{6}$$

and $\underset{\sim}{n}$ is the normal vector to the plane. We assume the dislocation glides freely unless pinned by obstacles.

Let the gliding dislocation encounter two impenetrable point obstacles. The dislocation segment between the obstacles bows out to an equilibrium radius[2]

$$R = {}^{\Gamma}/\tau b \tag{7}$$

if the obstacle separation is less than 2R. If the obstacle separation is greater than 2R the bowing segment is unstable, the dislocation folds around the obstacles to close on itself (the Orowan mechanism[3]) and the obstacles are mechanically bypassed.

Equation (7) suggests a useful non-dimensional measure of the stress impelling glide through an array of obstacles. We define the non-dimensional resolved shear stress

$$\tau^* = \tau l_s b/2\Gamma \tag{8}$$

or

$$\tau^* = l_s/2R = 1/2R^* \tag{9}$$

where R* is the dimensionless bow-out radius. Given this measure of stress, at $\tau^* = 1.0$ the dislocation will mechanically by-pass impenetrable obstacles separated by l_s. $\tau^* = 1.0$ is the critical resolved shear stress for dislocation glide through a square array of impenetrable point obstacles.

Now let the dislocation be pressed against a line configuration of point obstacles by the resolved shear stress τ^* (as, for example, in figure 1). Between each pair of adjacent obstacles the dislocation bows out to radius R*. If the distance between any two adjacent obstacles exceeds 2R* (= τ^{*-1}) or if the dislocation anywhere intersects itself, the particular configuration of obstacles is transparent to the dislocation and will be mechanically penetrated.

If the line configuration of obstacles is not transparent at applied stress τ^*, the dislocation line forms an angle $\psi (0 \leq \psi \leq \pi)$ at each point obstacle (figure 2). Let ψ_i^k be the angle formed at the k^{th} point obstacle in the i^{th} line configuration. The force which the dislocation line exerts on this obstacle is, as shown in the appendix,

$$F_i^k = 2\Gamma \cos (\psi_i^k/2). \tag{10}$$

Since Γ, the line energy of the dislocation, is a constant, we define the non-dimensional force

$$\beta_i^k = \cos (\psi_i^k/2). \tag{11}$$

The force β_i^k increases from 0 to 1 as the angle ψ_i^k decreases from π to zero. The mechanical force on the $i^{\underline{th}}$ configuration of obstacles is characterized by the set of dimensionless parameters $\{\beta_i^k\}$, where k takes on N_i values, one for each of the obstacles in contact with the dislocation along the $i^{\underline{th}}$ line. It is useful to order the $\{\beta_i^k\}$ so that β_i^k decreases with the index k. Given $\{\beta_i^k\}$ the line of obstacles may or may not be mechanically penetrated by the dislocation, depending on the strength of the obstacles.

The obstacles are assumed to be identical, circularly symmetric barriers to the dislocation. They are point obstacles in the sense that their range of effective interaction with the dislocation, of characteristic length d, is small compared to the mean obstacle separation l_s. As discussed in the appendix, the interaction of the obstacle with the dislocation may be treated as a point force on the dislocation line which may be made dimensionless through division by 2Γ. The total interaction is then represented by a force-displacement relation giving the point force on the dislocation as it sweeps through the obstacle (in dimensionless form, $\beta(^x/d)$). A force-displacement relation for a simple repulsive interaction is drawn schematically in figure 3.

The maximum (β_c) of the force-displacement relation ($\beta(^x/d)$) measures the effective mechanical strength of the obstacle. The obstacle (k,i) will be cut by the dislocation if $\beta_i^k < \beta_c$. Hence the $i^{\underline{th}}$ line configuration of obstacles is a mechanically stable barrier to the dislocation only if

$$\beta_i < \beta_c \tag{12}$$

where β_i is the largest member of the $\{\beta_i^k\}$. β_i is the force applied at the minimum angle (ψ_i) along the dislocation line.

If the inequality (12) is satisfied at every point along the $i^{\underline{th}}$ line configuration, and if we neglect the possibility of thermally-activated bow-out between adjacent obstacles, the dislocation remains pinned in this configuration until one obstacle is passed through thermal activation. The activation barrier which must be overcome to pass obstacle (k, i) is simply proportional to the area under the force-displacement curve ($\beta(^x/d)$) and above a horizontal line of height β_i^k (figure 3). If the function $\beta(^x/d)$ is monotonically increasing between the values β_i^k and β_c (we assume it is), the activation energy may be written in dimensionless form:

$$g_i^k = u(\beta_c) - u(\beta_i^k), \tag{13}$$

where $u(\beta)$ is the dimensionless area under both the force displacement curve and a horizontal line of height β. The activation barrier at obstacle (k, i) is then

$$\Delta G^{*k}_i = 2\Gamma d g_i^k. \tag{14}$$

III. THERMAL ACTIVATION PAST A LINE OF OBSTACLES

Given the activation energy (equation (14)) and neglecting any activation entropy, the stochastic probability for thermal activation past the (i, k) barrier in one attempt is

$$P_i^k = \exp\left(-\alpha g_i^k\right) \tag{15}$$

where g_i^k is given by equation (13) and α is a dimensionless reciprocal temperature

$$\alpha = {}^{2\Gamma d}/{}_{kT} \,. \tag{16}$$

The probability that the barrier remains uncut after j trials, given that it was intact initially, is

$$P_i^k\,(j) = [1 - P_i^k]^j \tag{17}$$

Let the dislocation attempt the obstacle with mean frequency ν, taken to be the same for all obstacles. Unless P_i^k is very small the activation probabilities are sensitive to the physical interpretation of ν. To be precise, let the activation trials occur randomly in time with expectation 1 per unit of dimensionless time

$$t^* = \nu t. \tag{18}$$

The probability of exactly j trials in time t* is then

$$P(j,t^*) = \frac{(t^*)^j}{j!} e^{-t^*} \tag{19}$$

and the probability that the obstacle is uncut at time t*, given that it was uncut at time zero, is

$$P_i^k\,(t^*) = \sum_{j=0}^{\infty} (j!)^{-1} (t^*)^j e^{-t^*}\,[1-P_i^k]^j$$

$$P_i^k\,(t^*) = \exp\left[-P_i^k\, t^*\right] \tag{20}$$

If the dislocation is pinned against the $i^{\underline{th}}$ obstacle configuration at $t^* = 0$, then all obstacles (k, i) on i are known to be uncut at $t^* = 0$, and we may compute the probability for activation past i without considering previous configurations or previous attempts to cut the obstacles on i (contrary to the statement of Argon[4], Arsenault and Cadman[5] and one of us in earlier work[6]). The probability that the $i^{\underline{th}}$ configuration remains uncut after time t^* is the probability that all obstacles on i remain intact at t^*:

$$P_i(t^*) = \prod_{k=1}^{N_i} P_i^k\,(t^*) = e^{-\Lambda_i t}, \tag{21}$$

where, from equation (20),

$$\Lambda_i = \sum_{k=1}^{N_i} P_i^k \tag{22}$$

The probability that the $i^{\underline{th}}$ configuration is cut in the time interval $(t^*, t^* + dt^*)$ is

$$P_i(t^*)dt^* = -\frac{\partial}{\partial t^*}\,(e^{-\Lambda_i t^*})\,dt^* = \Lambda_i e^{-\Lambda_i t^*} dt^* \tag{23}$$

Hence the expected residence time in the i^{th} configuration is

$$\langle t^*_i \rangle = \int_0^\infty t^* P_i(t^*)\,dt^* = \Lambda_i^{-1} \tag{24}$$

and the variance of the residence time is

$$\sigma_i^2 = \langle t_i^{*2} \rangle - \langle t_i^* \rangle^2 = \Lambda_i^{-2} \tag{25}$$

or

$$\sigma_i^2 = \langle t_i^* \rangle^2 \tag{26}$$

The expected residence time $\langle t_i^* \rangle$ is the mean time required for the dislocation to pass one obstacle in the $i^{\underline{th}}$ configuration. We may also compute the probability P(k, i) that the $k^{\underline{TH}}$ obstacle is the one passed. Let the $i^{\underline{th}}$ configuration be passed at time t*. Then

$$P(k,i|t^*) = \left[P_i^k \, e^{-P_i^k t^*}\right]\left[\prod_{k \neq i = 1}^{N_i} \exp(-P_i^j t^*)\right] = P_i^k \, e^{-\Lambda_i t^*} \quad (27)$$

where the first bracketed term is the probability that obstacle k is passed at time t* and the second bracketed term is the probability that all other barriers remain. It follows that

$$P(k,i) = P_i^k \int_0^\infty e^{-\Lambda_i t^*} \, dt^* = P_i^k / \Lambda_i \quad (28)$$

As is apparent from equations (15) and (22) Λ_i will in general be a rather complicated function of temperature even if the applied stress (and hence the $\{g_i^k\}$) is held constant. Barring the trivial case in which the g_i^k are identical, as for a straight line of equispaced obstacles, it will generally not be possible to write Λ_i in the form of a simple Arrenhius equation with a constant activation energy. However, in the limiting cases of small α (high temperature) and large α (low temperature) Λ_i does simplify to an Arrenhius form.

As the temperature T is made large α approaches zero. Hence there is a range of α such that

$$\alpha \, g_i^{N_i} << 1 \quad (29)$$

where $g_i^{N_i}$ is the largest member of $\{g_i^k\}$. This range of α will, however, fall at unrealistically high temperatures unless $g_i^{N_i}$ is small; α (equation (16)) has a realistic minimum of about 10 at the melting point of a typical metal. When the inequality (29) is satisfied,

$$\Lambda_i \cong \sum_{k=1}^{N_i} (1 - g_i^k) \sim N_i e^{-\alpha \bar{g}_i} \tag{30}$$

where $\bar{g}_i$ is the average value of g_i^k. The mean residence time is then

$$<t^*_i> = \frac{1}{\bar{N}_i} e^{\alpha \overline{g_i}} . \tag{31}$$

as would obtain from a simple activation process with N_i paths in parallel, each of which has dimensionless activation energy $\overline{g_i}$. The probability that the $k^{\underline{th}}$ obstacle is the one passed approaches $(1/N_i)$, consistent with this point of view.

As the temperature is decreased α increases without bound. If N_i is finite and if $g_i^2 - g_i^1$ is non-zero (i.e., if the weakest point in the barrier configuration is weaker than any other by a finite amount) then there is a range of α so large that

$$\alpha >> \ln N_i / g_i^2 - g_i^1 \tag{32}$$

When this condition obtains

$$\Lambda_i = e^{-\alpha g_i^1} \left[1 + \sum_{k=2}^{N_i} e^{-\alpha (g_i^k - g_i^1)} \right] \cong e^{-\alpha g_i^1} \tag{33}$$

Then

$$<t_i^*> \cong e^{\alpha g_i^1} \tag{34}$$

as expected for a simple activation process with a single path having activation energy g_i^1. Consistent with this point of view

$$P(k,i) \cong \delta_{k1} \tag{35}$$

and the $i^{\underline{th}}$ configuration is virtually certain to be passed at its weakest point, i.e., where the dislocation forms the minimum angle, ψ_i.

Finally, when N_i is large and the g_i^k are densely distributed over the domain $g_i^1 \le g \le g_i^{N_i}$, we may define a density function $\rho_i(g)$, the fraction of the g_i^k in dg at g and write

$$\Lambda_i = N_i \int_0^\infty e^{-\alpha g} \rho_i(g)dg = N_i L_i(\alpha) \tag{36}$$

where $L_i(\alpha)$ is the LaPlace transform of the density function $\rho_i(g)$. $L_i(\alpha)$ is the average value of the P_i^k on i and is non-zero for finite α. As N_i becomes arbitrarily large at fixed $\rho_i(g)$, Λ_i increases without bound and $\langle t_i^* \rangle$ approaches zero. However, it does not follow that the distinction between obstacle configurations is negligible when the number of obstacles on a line is large. Given two configurations i and j with $N_i \approx N_j$ but $\rho_i(g) \neq \rho_j(g)$ the ratio of residence times is

$$\langle t_i^* \rangle / \langle t_j^* \rangle = {}^{L_j(\alpha)}/{}_{L_i(\alpha)} \tag{37}$$

when N_i is arbitrarily large. This ratio may differ markedly from one.

IV. THE TRANSIT TIME FOR GLIDE THROUGH AN ARRAY OF OBSTACLES

Let a dislocation glide through a finite array of randomly distributed point obstacles at given values of τ^* and α. We assume the process is controlled by thermal activation in the sense that the time required for glide between mechanically stable configurations is negligible compare to the time required for thermal activation.

The statistics of thermally activated glide are complicated by the fact that, except in certain limiting cases discussed below, the sequence of stable configurations encountered by the dislocation is not unique. At fixed temperature and stress a dislocation pinned by the $j^{\underline{th}}$ stable configuration may activate at any one of the obstacles (k,j) on j. The future path of the dislocation will in general depend on which specific obstacle is cut. The problem is, however, somewhat simplified by the fact that the configurations assumed in glide through a finite array form an irreducible Markov chain (ref. 7, Chapt. XV).

Let the dislocation be in its $j^{\underline{th}}$ stable configuration, and let point (k,j) be cut through thermal activation. The subsequent glide of the dislocation is governed by its mechanical equations of motion and continues until a new stable configuration, the $(j + 1)^{\underline{th}}$, is reached. The $(j + 1)^{\underline{th}}$ configuration is thus uniquely determined by the $j^{\underline{th}}$ configuration and by the activation site (k,j). The probability that a particular configuration (i) will be the $(j + 1)^{\underline{th}}$ is known once the $j^{\underline{th}}$ configuration is known, independent of previous events, and is simply the probability that activation will occur at a point on j (there may be several) which causes j to evolve into i. Hence the activation process in Markovian.

Let χ be a path through the array, i.e., a possible sequence of configurations assumed as the dislocation glides through the array. The first member of χ must necessarily be the first stable configuration encountered as the dislocation moves into the array. Let {q}, with q elements, be the set of all stable configurations which can be reached from this initial position by activating past obstacles in any sequence. Since the array is finite, q is finite. The elements of {q} form a

Markov chain which is irreducible since any member of $\{q\}$ may be reached by thermal activation and hence may lie on the particular path taken by the dislocation. It follows from the ergodic property of such chains (ref. 7, section XV. 6) that the probability P_χ that the dislocation takes path χ is defined, and

$$\sum_\chi P_\chi = 1 \tag{37}$$

The probability P_i that the dislocation encounters configuration i is the sum of P_χ over all paths which contain i

$$P_i = \sum_\chi P_\chi \tag{38}$$

and

$$r = \sum_{i=1}^{g} P_i \tag{39}$$

is the expected number of stable configurations encountered. Given equation (28), however, both P_χ and P_i may be complex functions of stress, temperature, and the nature of the obstacles. The set $\{q\}$ itself is a function of dimensionless stress, even if the nature of the obstacles is fixed.

Let the dislocation follow a particular path χ through the array and let χ contain r configurations having activation parameters Λ_i $(i = 1,\ldots,r)$. The time t* required for glide through the array is then the sum of r random variables t_i^* $(i = 1,\ldots,r)$ distributed according to r density functions $P_i(t^*)$, where $P_i(t^*)$ is defined in equation (23). It follows (ref. 7, Chapt. IX) that the expected value of t* is

$$<t^*_\chi> \;=\; \sum_{i=1}^{r} <t^*_i> = \sum_{i=1}^{r} (\Lambda_i)^{-1} \tag{40}$$

and that the variance of σ^2_χ of t* is

$$\sigma^2_\chi = \sum_{i=1}^{r} \sigma^2_i = \sum_{i=1}^{r} (\Lambda_i)^{-2} \tag{41}$$

The random variables t^*_i may be shown to obey the conditions of the Lindeberg theorem (ref. 7, p. 239). Hence as r becomes large the distribution of t* approaches a normal distribution with the density function

$$p(t^*_\chi) = (2\pi\sigma^2_\chi)^{-1/2} \exp - \frac{(t^* - <t^*_\chi>)^2}{2\sigma^2_\chi} \tag{42}$$

giving the probability that t^*_χ lies in the range (t*, t* + dt*).

Using equations (40) and (41)

$$\sigma^2_\chi/<t^*_\chi> = \left\{ 1 + \left[2 \sum\sum_{i<j=1}^{r} (\Lambda_i\Lambda_j)^{-1} \right] \left[\sum_{i=1}^{r} \Lambda_i^{-2} \right]^{-1} \right\}^{-1} \tag{43}$$

Let Λ^χ_o be the minimum value of Λ_i encountered along path χ. When the number of configurations having Λ_i near Λ^χ_o is large the ratio (43) is small and the transit time t^*_χ for transit via path χ is very likely to be within a few percent of the expected value $<t^*_\chi>$. As we shall illustrate in paper II this condition may fail when the stress τ^* is very close to τ^*_c, since r is then small, or when the reciprocal temperature α is large, since the number of Λ_i near Λ^χ_o is then small. In either of these cases the scatter in t^*_χ may be large.

Given equations (37), (38), and (41) the time t^* to transit a random array is distributed according to the density function

$$p(t^*) = \sum_{\chi} p_{\chi}\, p(t^*|\chi) \tag{44}$$

with mean

$$\langle t^*\rangle = \sum_{\chi} p_{\chi} \langle t^*\rangle_{\chi} = \sum_{i=1}^{q} P_i \Lambda_i^{-1} \tag{45}$$

and variance

$$\sigma^2 = \sum_{\chi} p_{\chi} [\sigma_{\chi}^2 + (\langle t^*\rangle_{\chi} - \langle t^*\rangle)^2] \tag{46}$$

The expected value of the transit time is hence just the sum of the expected waiting times at the q possible configurations, weighted by the probabilities that they will lie along the dislocation path. The variance of the transit time is the weighted average of the sum of two independent variances: σ_{χ}^2, due to scatter in the waiting times for thermal activation along path χ, and $[\langle t^*\rangle_{\chi} - \langle t^*\rangle]^2$, due to the variation in expected transit time from one path to another. If the number of independent paths is large and the $\langle t^*\rangle_{\chi}$ are normally distributed about $\langle t^*\rangle$ the distribution of t^* will approach a normal distribution. Equation (44) may then be rewritten in the form (42) with mean $\langle t^*\rangle$ and variance σ^2. Similarly, if there is a unique path (χ_o) containing a sufficiently large number of configurations, the distribution of t^* is normal with mean $\langle t_o^*\rangle$ and variance σ_o^2.

There are two limiting cases in which one may reasonably assume a unique path for dislocation glide through the array. These cases are of particular interest since the assumption of a unique glide path greatly simplifies the activation process and makes it much more amenable to theoretical attack. χ becomes unique in the limit as $\alpha \to \infty$ or $\tau^* \to \tau_c^*$.

Let α be so large that the inequality (32) is satisfied for almost every configuration in $\{q\}$. It is then almost certain that the $i^{\underline{th}}$ stable configuration will be passed at its weakest point, where the dislocation forms the minimum angle ψ_i. Since at given stress the $(i + 1)^{\underline{th}}$ configuration encountered along the glide path is uniquely determined by the $i^{\underline{th}}$ and by point (k,i) at which activation occurs, the dislocation tends to follow a particular path χ_o, the "minimal sequence", obtained by constraining the dislocation to cut each stable configuration encountered at its weakest point.

If we assume that the dislocation follows path χ_o while always activating the minimum angle, we obtain an approximation (the "minimum angle approximation") which not only simplifies the problem but, as we have found(1), gives results which are reasonably accurate over a wide range of α and τ^*. The simplifications obtained are two. First, in this approximation the operational variables of the problem decouple. As follows from the discussion in Section II, the non-transparent configurations along χ_o are determined by the applied stress τ^*. Moreover, each of these lines is subjected to a maximum mechanical force β_1 which also depends on τ^* only. The stable configurations along χ_o at given stress are determined by the obstacle strength β_c according to the stability condition $\beta_1 < \beta_c$. The activation energy for cutting the $i^{\underline{th}}$ stable configuration is g_i^1, determined from the force-displacement diagram by equation (13). Temperature then enters only in determination of the transit time. Assuming a large number (r_o) of stable configurations along χ_o, t^* is normally distributed with mean

$$t^* = \sum_{i=1}^{r_o} e^{\alpha g_i^1} \tag{47}$$

and variance

$$\sigma_o^2 = \sum_{i=1}^{r_o} e^{2\alpha g_i^1} \tag{48}$$

Similar results follow in the limit $\tau^* \sim \tau_c^*$. In this limit the dislocation tends to follow χ_o independent of temperature. As τ^* increases the number of stable lines decreases until eventually there is only one stable configuration in the array, the configuration which determines τ_c^*. Barring the possibility of a serious overlap of very strong configurations there will, therefore, be a stress τ^* so large that almost all stable lines are spatially separated from one another in the sense that they have no obstacle points in common. In this limit every point in the $i^{\underline{th}}$ stable line configuration will be passed mechanically ("unzipped" in the terminology of Dorn, et al[(8)]) once any single point is passed by thermal activation. Since the dislocation can only pass a stable configuration by thermal activation, the $(i + 1)^{\underline{th}}$ configuration is uniquely determined by the $i^{\underline{th}}$ irrespective of the activation site (k,i). The dislocation then follows the glide path χ_o.

This limiting case suggests an approximation (the "minimal sequence approximation") in which we constrain the dislocation to follow the path χ_o, but employ statistically correct activation parameters Λ_i. The operational variables again decouple. The stable configurations along χ_o are determined by τ^* and β_c as described above. The activation energies in the $i^{\underline{th}}$ configuration, $\{g_i^k\}$, are determined from the force displacement diagram. The parameters Λ_i are determined from the g_i^k and α according to equations (15) and (22). Assuming a large number of stable lines t^*

is normally distributed with mean and variance given in terms of the Λ_i by equations (40) and (41).

The equations derived in this section show that <t*> is a complex function of α which cannot be obviously represented by an equation of the Arrenhius form. The equation governing <t*> may, however, reduce to a simple Arrenhius form in the limits of large α (low temperature) and small α (high temperature).

Let α be so large that the minimum angle approximation applies (equation 47). Let g_o and g_1 be respectively the largest and second largest members of $\{g_i^1\}$, and assume that they differ by a finite amount. Since α increases without bound as temperature approaches zero, there will be a range of α over which

$$\alpha \gg \ln (r_o)/g_o - g_1 \tag{49}$$

In this limit

$$\langle t^* \rangle \approx e^{\alpha g_o} \tag{50}$$

an equation of the Arrenhius form with activation energy g_o.

Now, recalling equation (30), let α be so small that $\alpha\bar{g}_i$ is much less than one, and the condition (29) is satisfied for every configuration in $\{q\}$. In this limit all obstacles in a given configuration have almost equal probability of being passed, and P_χ and hence P_i approach limiting values. It then follows from equations (30) and (45) that

$$\langle t^* \rangle \cong A_o e^{\alpha\bar{g}} \tag{51}$$

an equation of the Arrenhius form with

$$A_o = \sum_{i=1}^{q} P_{i/N_i} \tag{52}$$

and

$$\bar{g} = A_o^{-1} \sum_{i=1}^{q} (P_i/N_i)\, \bar{g}_i \tag{53}$$

V. THE VELOCITY OF GLIDE THROUGH A GIVEN ARRAY OF OBSTACLES

As may be inferred from the equations presented in the preceeding sections, and as we shall show through specific examples[1], the glide of a dislocation through a random array of obstacles is not smooth. A dislocation spends a majority of its transit time pinned by the stronger obstacle configurations and jumps rapidly through weak intervening configurations when it has activated past a strong stable configuration. As a consequence, the velocity of glide is defined only in a statistical sense.

We define the expected value of the velocity of glide through a given array of obstacles in the following way. Imagine a crystal made up of an ensemble of parallel glide planes which replicate the given array. Let a distribution of non-interacting gliding dislocations be distributed through the crystal. The expected value of the instantaneous rate of strain of the crystal is

$$\dot{\gamma} = \frac{b}{V}\left\langle \partial A/\partial t \right\rangle \tag{54}$$

where $\langle \partial A/\partial t \rangle$ is the expected total area swept per unit time and V is the volume of the crystal. This equation may be rewritten

$$\dot{\gamma} = \rho b \langle v^* \rangle \tag{55}$$

where ρ is the density of dislocations and $\langle v^* \rangle$ is the expected value of the dimensionless velocity:

$$\langle v^* \rangle = n^{-1/2} \langle \dot{a}^* \rangle \tag{56}$$

where n is the number of obstacles in the array, $n^{1/2}$ is the dimensionless edge length of the array and $\langle \dot{a}^* \rangle$ is the expected value of the (dimensionless) areal velocity per dislocation. $\langle v^* \rangle$ is hence the expected value of the area swept out per dislocation per unit time divided by the projected length of the dislocation.

The expected value $\langle \dot{a}^* \rangle$ is easily found from the equations of section IV. The fraction (f_i) of the dislocations in an ergodic distribution positioned in configuration i at a given instant of time is equal to the fraction of time a given dislocation spends in configuration i during an arbitrarily large number of sequential passages through the same array. From equation (45) this fraction is

$$f_i = {}^{P_i}/\Lambda_i \langle t^* \rangle \, . \tag{57}$$

The probability that a dislocation will activate past configuration (i) in incremental time δt^* is, from equation (23),

$$P_i(\delta t^*) = \Lambda_i \delta t^* \tag{58}$$

Let a_i^* be the dimensionless area swept out when the $i^{\underline{th}}$ configuration is passed. Then

$$\langle \dot{a} \rangle = \lim_{\delta t^* \to o} \frac{1}{\delta t^*} \left\{ \sum_{i=1}^{q} f_i P_i(\delta t^*) \, a_i^* \right\}$$

$$= \frac{1}{\langle t^* \rangle} \sum_{i=1}^{q} P_i a_i^* \tag{59}$$

If the array is large enough that we may neglect end effects, the dislocation sweeps out dimensionless area n in passing through the array. Hence, the summation in equation (59) is equal to n and

$$\langle \dot{a}^* \rangle = {}^{n}/\langle t^* \rangle , \tag{60}$$

that is, $\langle \dot{a}^* \rangle$ is equal to the area of the glide plane divided by the expected transit time. The expected value of the velocity is

$$\langle v^* \rangle = n^{1/2} / \langle t^* \rangle \tag{61}$$

the length of the array divided by the expected transit time.

Equations (60) and (61) show that the expected value of the velocity may be easily computed from the expected value of the transit time. If the array is large and well-behaved so that the transit time t^* is normally distributed and the ratio $\sigma^2/\langle t^* \rangle^2$ is small, the expected glide velocity may be estimated from the actual transit time for a single passage. Defining the apparent areal velocity

$$\dot{a}^* = n / t^* \tag{62}$$

and the parameter δ,

$$\delta = (\dot{a}^* - \langle \dot{a}^* \rangle) / \langle \dot{a}^* \rangle, \tag{63}$$

the fractional deviation of $\dot{a}^*$ from its expected value, it follows from the normal distribution of t^* that values of δ near zero are normally distributed according to the density function

$$p(\delta) = (2\pi)^{-1/2} (\langle t^* \rangle / \sigma) \exp \left\{ - \frac{1}{2} (\langle t^* \rangle / \sigma)^2 \delta^2 \right\} \tag{64}$$

This distribution has mean zero and variance $\sigma^2/\langle t^* \rangle^2$. As $\sigma^2/\langle t^* \rangle^2$ approaches zero a measured value $\dot{a}^*$ is almost certain to differ from $\langle \dot{a}^* \rangle$ by no more than a small fraction.

Given equation (61), it follows that $\langle v^* \rangle$ will obey an equation of the Arrenhius form

$$\langle v^* \rangle = A e^{-\alpha g} \tag{65}$$

only when $\langle t^* \rangle$ does. Following the discussion of section IV when α is so large (temperature so low) that the condition (49) is obeyed, $\langle v^* \rangle$ obeys an Arrenhius equation with $A = n^{1/2}$ and $g = g_o$. When α is sufficiently small (temperature high), $\langle v^* \rangle$ obeys an Arrenhius equation with $A = n^{1/2} A_o$ and $g = \bar{g}$ (equation 51). In general, however, an attempt to fit $\langle v^* \rangle$ to an Arrenhius equation will result in parameters A and g which are functions of α.

VI. GLIDE VELOCITY IN A SIMPLE CRYSTAL

Suppose a crystal is made up of a large number of parallel glide planes of equal dimensionless area (n) which contain independent distributions of idential obstacles. The expected glide velocity $\langle v^* \rangle$, as defined by equation (56), may vary from plane to plane. There are two possible sources of variation: the number of obstacles in the plane, and the distribution of these obstacles.

Given a stochastic distribution of points over a plane the probability that a dimensionless area (n) will contain exacly j points is given by the Poisson formula

$$P(j) = \left(\frac{n^j}{j!}\right) e^{-n} \tag{63}$$

The mean value of j is n, but its variance is also n. Hence, unless n is large, the percentage scatter in the number of points from plane to plane will be appreciable. As follows from section II, a decrease in the number of points randomly distributed over a plane of fixed area is equivalent to an increase in the dimensionless applied stress at given actual stress. Since the glide velocity depends on the dimensionless stress, a scatter in the number of points per plane will induce a scatter in the glide velocity per plane.

The statistical scatter in the number of points per plane becomes less pronounced as the area of the plane increases. When n is large, one may define the fractional deviation

$$\delta_n = {}^{j-n}/_{n} \tag{64}$$

and use the normal approximation to the Poisson distribution to show that δ_n is distributed according to the density function

$$P(\delta_n) \cong ({}^{n}/2\pi)^{1/2} \exp -(\tfrac{n}{2})\, \delta_n^{\,2} \tag{65}$$

The variance of δ_n, n^{-1}, approaches zero with increasing n.

The second source of scatter in <v*> is the stochastic variation in the precise distribtuion of points from plane to plane. As shown in section IV, except, possibly, in the high temperature limit <t*> and σ^2 are sensitive to the distribution of stable obstacle configurations, and hence to the distribution of points over the plane. In the second paper of this series we shall show[1] the plane-to-plane variation of <v*> using a particular model and fixing the number of points per plane at 999. In this case the scatter in <v*> is noticeable. It seems plausible that scatter due to obstacle distribution will also vanish as the area n is made arbitrarily large; however, a proof requires a sound theory of obstacle configurations, now unavailable.

The average velocity of dislocation glide in the crystal may be defined in either of two ways: (1) from the strain rate due to a distribution of gliding dislocations, as in equation (55), or (2) as the expected velocity for glide through a randomly chosen plane. If the planes are finite these two definitions are not formally equivalent.

First, let an ensemble of non-interacting dislocations be ergodically distributed through the crystal. The expected fraction of these dislocations ($f_{i,l}$) located at the $i^{\underline{th}}$ configuration of the $l^{\underline{th}}$ plane at a given instant of time is equal to the fraction of time a single dislocation would spend in [i,l] if it sequentially traversed all planes a large number of times. Using equation (57),

$$f_{i,l} = P_{i,l}/\Lambda_{i,l} S\bar{t}^* \tag{66}$$

where S is the number of planes and

$$\bar{t}^* = \frac{1}{S} \sum_{l=1}^{S} \langle t^* \rangle_l \tag{67}$$

is the average time to transit an array. It follows from a derivation identical to that giving equation (61) that

$$\bar{v}^* = n^{1/2}/\bar{t}^* \tag{68}$$

where $\bar{v}^*$ is the average velocity determined from the strain rate.

Alternately, let $\tilde{v}^*$ be the average of the velocity of glide through a randomly chosen plane. Then

$$\tilde{v}^* = n^{1/2}\, \overline{(t^*)^{-1}} \tag{69}$$

where

$$\overline{(t^*)^{-1}} = \frac{1}{S} \sum_{l=1}^{S} \langle t^* \rangle^{-1} \tag{70}$$

is the average reciprocal transit time, which may differ markedly from the reciprocal of the average transit time. Hence $\bar{v}^*$ and $\tilde{v}^*$ are not necessarily equivalent measures of the average velocity.

The velocities $\bar{v}^*$ and $\tilde{v}^*$ are nearly equal if almost all planes in S have transit times very close to $\bar{t}^*$. Mathematically, $\bar{v}^* \approx \tilde{v}^*$ if the variance Σ^2 of t^* for a randomly chosen plane of the crystal,

$$\Sigma^2 = \frac{1}{S}\sum_{l=1}^{S}\left\{\sigma_l^2 + (\langle t_l^*\rangle - \bar{t}^*)^2\right\} \tag{72}$$

satisfies the constraint

$$\Sigma^2/(\bar{t}^*)^2 \ll 1 \tag{73}$$

VII. DISCUSSION

The relations developed in the proceeding sections significantly reduce the theoretical or numerical work necessary to obtain a reasonably complete solution for thermally activated glide through an array of identical point obstacles. The simplification is particularly great when either the minimal sequence or minimum angle approximation is used. Given a numerical code which simulates dislocation glide one may proceed as follows:

The glide of an idealized dislocation through a given distribution of point obstacles depends on three dimensionless parameters: the resolved stress (τ^*), the reciprocal temperature (α), and the dislocation obstacle interaction $\beta(^x/d)$. Given these parameters, let the code introduce a dislocation into the array and let the dislocation glide until a mechanically stable configuration is found. Let the code find the angle ψ_i^k at each point obstacle along this line configuration. The forces β_i^k, are then computed from equation (11) and the activation energies, g_i^k, are found from the β_i^k and the dislocation-obstacle interaction according to equation (13). Given α, the activation probabilities, P_i^k, are computed from equation (15) and the activation parameter Λ_i is found from equation (22). Now let an activation site be selected according to the probability distribution (28). When this obstacle is passed the dislocation finds a new stable configuration (i + 1). Λ_{i+1} may be computed and activation repeated to obtain (i + 2). Iteration leads to glide through the array along a statistically chosen path (χ). The expected value $\langle t^* \rangle_\chi$ of the transit time t^* is given in terms of Λ_i by equation

(40) and the variance, σ_χ^2, of t^*_χ is determined by equation (41). If the number of configurations in χ is large t^*_χ is normally distributed according to equation (42). Hence the statistics of thermal activation along a glide path χ containing a large number of configurations may be found from a single numerical "experiment".

To obtain the complete statistics of thermally activated glide through the array, we strictly require knowledge of all paths χ and their probabilities P_χ. However, if the glide is well-behaved we should obtain a reasonable estimate of the distribution of the transit time t* by conducting a few (say h) independent experiments and computing the mean, the variance, and the distribution of t* from the appropriate modifications of equations (45), (46), and (44):

$$<t^*> = \frac{1}{h} \sum_{\chi=1}^{h} <t^*>_\chi$$

$$\sigma 2 = \frac{1}{h} \sum_{\chi=1}^{h} \left[\sigma_\chi^2 + (<t^*> - <t^*>)^2 \right]$$

$$p(t^*) = \frac{1}{h} \sum_{\chi=1}^{h} p(t^*|\chi).$$

The expected value of the glide velocity, <v*>, is then given in terms of <t*> and the array size n by equation (61). The statistics of activated glide through a distribution of obstacle arrays may be estimated by repeating these numerical trials for a series of independently chosen obstacle distributions.

Much of the complication faced in computing the statistics of glide through a given array comes from the indeterminacy of the glide path χ and the fact that the probability of a particular path depends on all three of the operational parameters of the problem. This complication is removed when the unique "minimal path" χ_o is assumed through use of either the minimal sequence or minimal angle approximations discussed in Section IV. χ_o is a function of the stress τ^* only. Hence in either the minimal sequence or the minimum angle approximation the statistics of glide may be computed for arbitrary α and $\beta(^x/d)$ from the results of a single numerical experiment at stress τ^*.

To use the minimal sequence approximation, given τ^* set $\beta_c = 1.0$ and let the dislocation glide through the array under the constraint that activation always occurs at the minimum angle ψ along the dislocation line. This constraint generates the path χ_o. Let the forces $\{\beta_i^k\}$ be tabulated for each non-transparent line encountered along χ_o. Now assume an arbitary dislocation-obstacle interaction $\beta(^x/d)$ having maximum β_c. The mechanically stable lines along χ_o are determined from β_c by the condition (12) and the activation parameters $\{g_i^k\}$ for these stable lines are given in terms of $\beta(^x/d)$ by equation (13). Given an arbitary value of α the P_i^k are computed from equation (15) and the Λ_i from equation (22). The full statistics of thermally activated glide through the array are then easily found.

The average velocity $\bar{v}^*$ of glide through a distribution of S arrays at given τ^*, but arbitrary α and $\beta(^x/d)$, may also be computed from a single numerical experiment when the minimal sequence approximation is used. Given τ^*, one finds the minimal path χ_o for sequential glide through the S arrays in random order. Once the $\{\beta_i^k\}$ have been tabulated for all non-transparent lines along χ_o the expected time $(S\bar{t}^*)$ to transit χ_o may be easily computed for given α and $\beta(^x/d)$. The velocity $\bar{v}^*$ is then given by equation (68).

Computations using the minimum angle approximation are identical to those using the minimal sequence approximation with the further simplification that one need only tabulate the maximum (β_i) of the $\{\beta_i^k\}$ for each non-transparent configuration in χ_o.

ACKNOWLEDGEMENT

This work was supported by the U. S. Atomic Energy Commission through the Inorganic Materials Research Division of the Lawrence Berkeley Laboratory.

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APPENDIX

While equation (10) appears frequently in the literature, its validity as a measure of the force exerted on a dislocation by a circularly symmetric point obstacle has been questioned by Kocks[9]. We append the following derivation.

Let the dislocation-obstacle interaction be circularly symmetric in the glide plane and have an effective range (d') which is very small compared to the characteristic length (l_s) of the array. Consider a portion of a dislocation pressed against a single obstacle by an applied stress τ^*. An equilibrium configuration of the dislocation line will appear roughly as shown in figure A1. The total energy of this configuration may be written

$$E = \int_L \Gamma dl + \tau b A_L + W \tag{A1}$$

where Γ is the line energy of the dislocation and the integral is taken over the portion (L) of the dislocation line included in the figure; A_L is the area behind L and $\tau b A_L$ measures the potential energy of L under stress τ; and W is the total energy of the interaction of L with the obstacle.

Using a two dimensional form of Gibbs[10] construction (illustrated in figure A1) the obstacle may be formally reduced to a point and the energy W localized. Given that d' is small we enclose the obstacle in an imaginary circle (D) of small radius d appreciably greater than d'. Only the portion of L within D is perturbed by the obstacle. We then extrapolate the two arms of L into D until they meet at a point (x). Let the extrapolated lines represent the dislocation within D and let the point of intersection represent the obstacle. The total energy of this hypothetical configuration (L') is

$$E' = \int_{L'} \Gamma dl' + \tau b A_{L'} + W', \tag{A2}$$

which is identical to E if

$$W' = W + \int_{D} \left\{ \Gamma(dl - dl') + \tau b\ (dA_L - dA_{L'}) \right\} \tag{A3}$$

If the dislocation is in mechanical equilibrium, then there must be no possible variation of L (or, equivalently, of L') which causes the energy to decrease. As may be easily seen by considering variations which leave the position of the point (x) in L' unchanged, it is necessary for equilibrium that W' have its minimum value, W'(x), consistent with the position (x) and the configuration of L outside of D, and that L' be symmetric about a line (l) through x and the physical center of the obstacle. If L' satisfies these conditions and if it is in equilibrium with respect to all variations which carry x along l and constrain W' to W'(x), then it is in equilibrium with respect to any variation whatever. Hence from equation (A2), L' is in mechanical equilibrium only if

$$\delta E' = \int_{L} ({}^{\Gamma}/R - \tau b)\delta x_n\ dl' + \left({}^{dW'}/dx_l - 2\Gamma \cos {}^{\psi}/2\right)\delta x_l \geq 0 \tag{A4}$$

In this equation R is the radius of curvature of the element dl' of L and δx_n is the normal displacement of this element. The angle ψ is the angle formed by L' at the intersection point x and the term involving ψ accounts for the net change in line length L' due to the displacement δx_1 of x along 1.

Since the infinitesimal displacements δx_n and δx_1 are independent and may have either sign, the inequality (A4) yields two necessary conditions for equilibrium:

$$(1) \quad \tau b = {}^{\Gamma}/_{R} \tag{A5}$$

everywhere on L' and

$$(2) \quad F = {}^{dW'}/dx_1 = 2\Gamma\cos{}^{\psi}/2 \tag{A6}$$

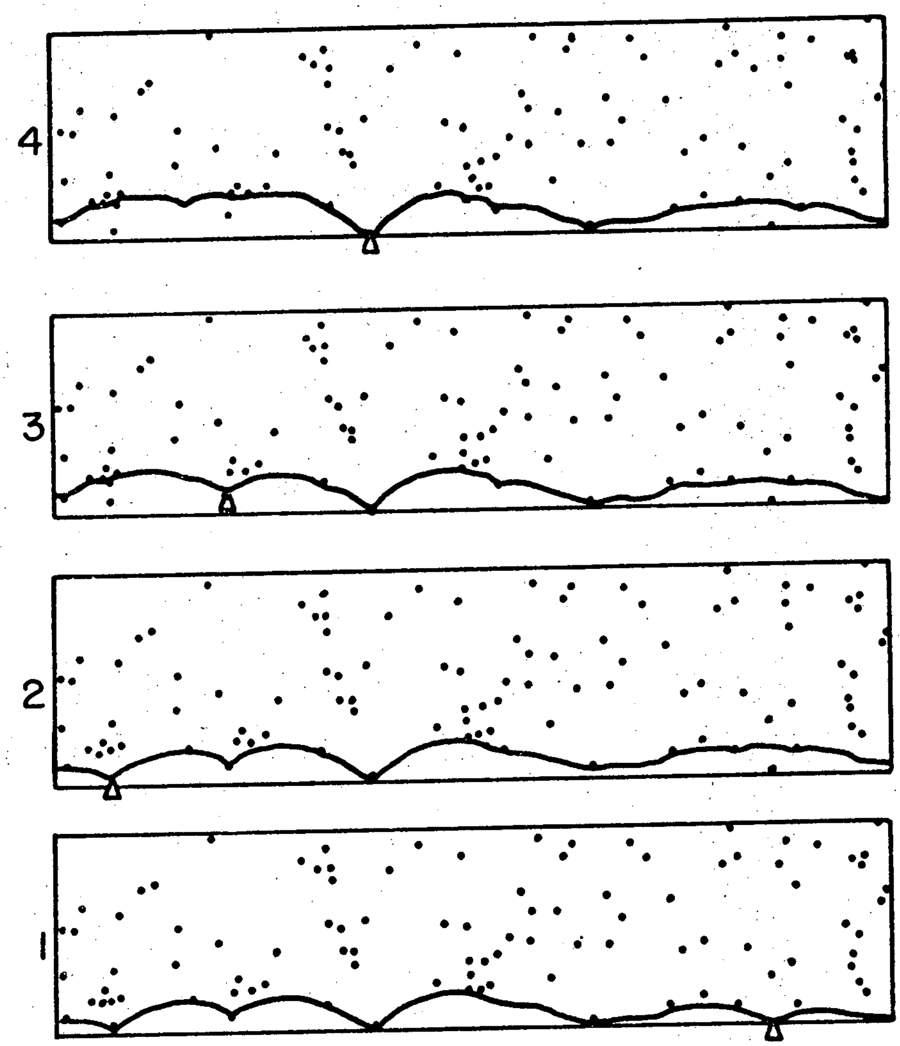
at the intersection point x. Condition (1) is identical to equation (7) of section II; condition (2) is identical to equation (10).

The force F is given as a function of the distance x_1 along the easiest cutting direction by equation (A6). This equation leads to the obstacle force-displacement relations discussed in section II. The meaningful values of x_1 cover an interval of maximum width 2d. The obstacles are point obstacles in the sense that d is small compared to the characteristic length l_s.

FIGURE CAPTIONS

1. Sequence of four possible configurations as a dislocation glides into a random array of point obstacles. The activation site is indicated by the symbol (Δ).
2. Detail of equilibrium in the $i^{\underline{th}}$ configuration.
3. A possible force-displacement relation, $\beta(^{x}/d)$, for dislocation passage through an obstacle which forms a simple repulsive barrier. The shaded area indicates the activation energy (g_i^k) if the disloca- exerts a force β_i^k on the obstacle.

A1. An illustration of the geometric construction used to define the point properties of an obstacle having a circularly symmetric interaction with a dislocation.



XBL732-5722

Fig. 1

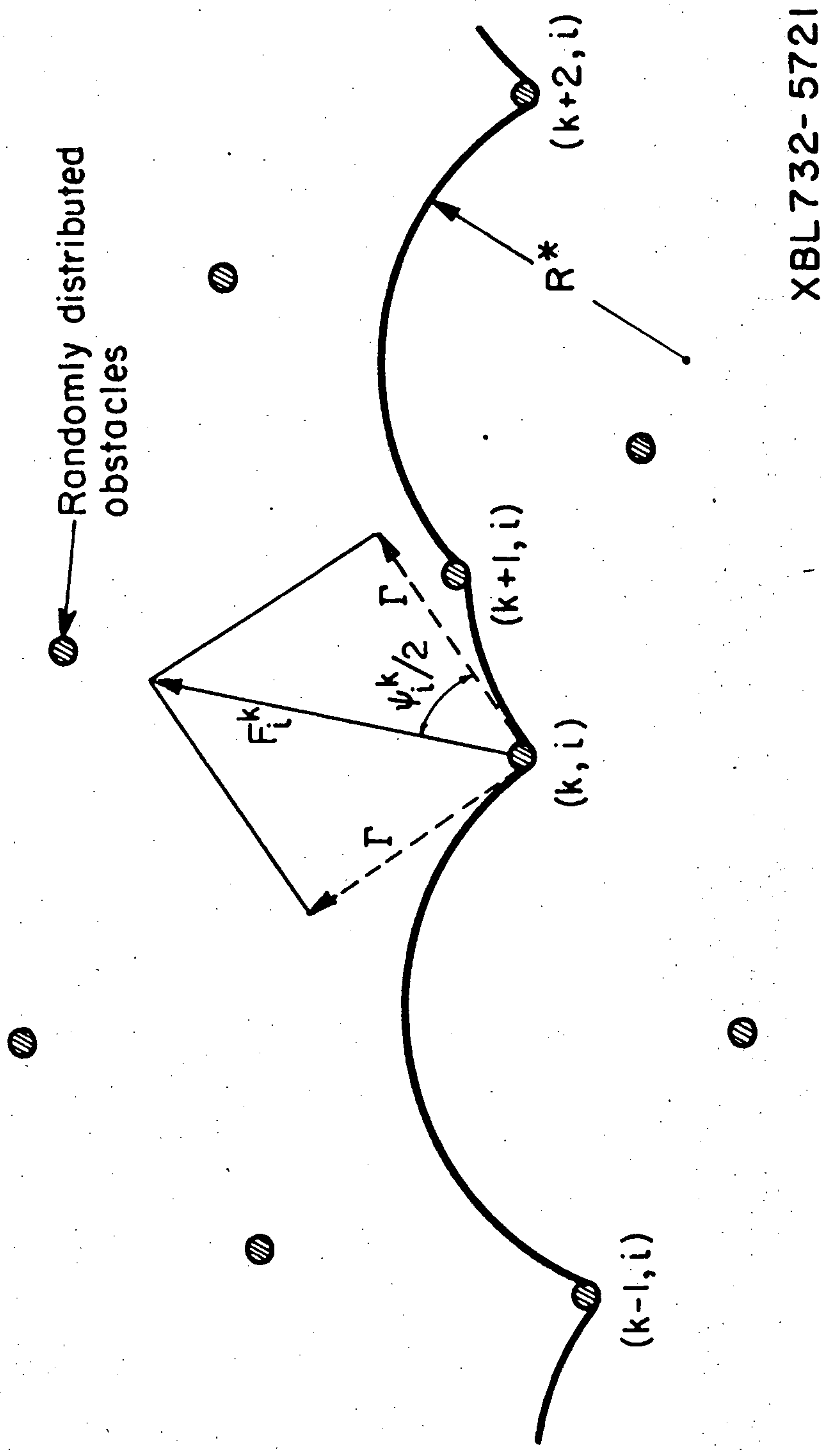

Randomly distributed obstacles
(k+2, i)
R*
(k+1, i)
Γ
ψ_i^k/2
F_i^k
(k, i)
Γ
(k-1, i)
XBL 732-5721

Fig. 2

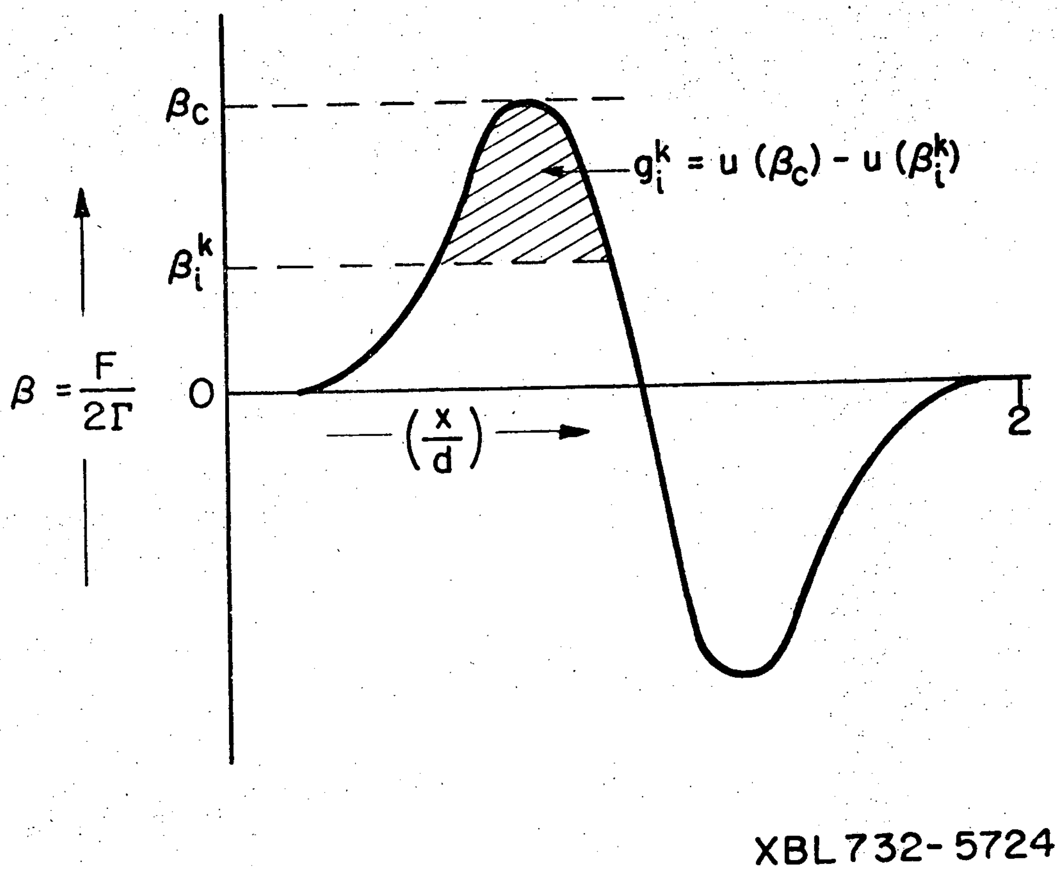

β_c
$g_i^k = u(\beta_c) - u(\beta_i^k)$
β_i^k
$\beta = \frac{F}{2\Gamma}$
0
$\left(\frac{x}{d}\right)$
2
XBL 732-5724

Fig. 3

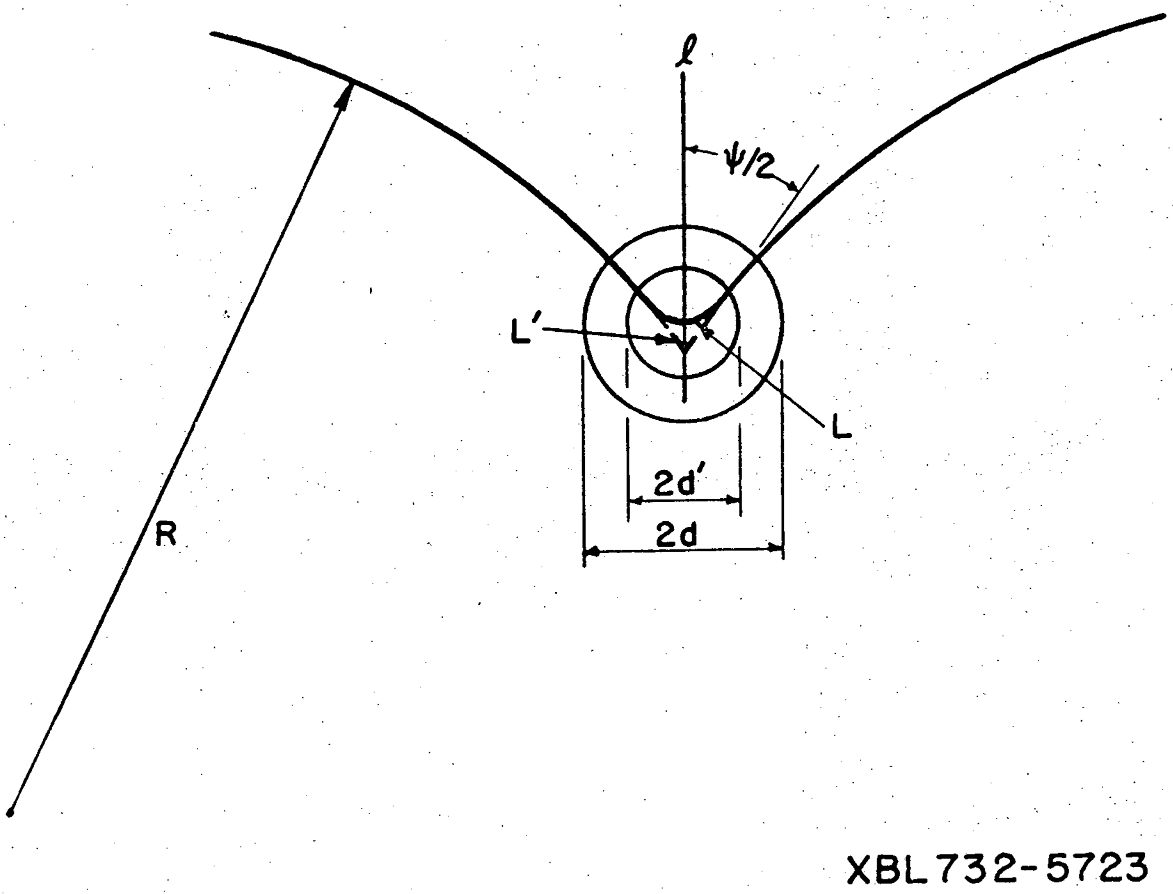


Fig. A1

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LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720