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RANDOM ARRAY OF OBSTACLES

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CHARACTERISTICS OF DISLOCATION GLIDE THROUGH A RANDOM  
ARRAY OF OBSTACLES

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ABSTRACT

This paper discusses characteristics of 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. Two characteristics of the motion are emphasized. First, the glide is jerky. The degree of this "jerkiness" is principally determined by temperature. Second, the velocity of glide at low to moderate temperature can be fit to an equation of the Arrhenius type only if a pre-exponential function of temperature and stress is incorporated.

## 1. 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 more or less in a random fashion through the structure. 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 study relies on computer simulation and statistical analysis. The computer code and initial results are discussed elsewhere<sup>1,2</sup>. In the present paper we emphasize two results of this study which may have important physical meaning.

First, the motion of a dislocation through a finite random array of point obstacles is usually jerky. A few positions within the array efficiently pin the dislocation for times long compared to the transit times between these "strong" configurations. Consequently, the dislocation appears to jump almost discontinuously from one of these configurations to another. The degree of this "jerkiness" is principally determined by the temperature. The "jerkiness" also tends to increase with applied stress, but stress is the dominant variable only when the temperature is very high, the obstacle strength is very low, or the stress is very close to the zero-degree yield stress of the array.

Second, the dependence of dislocation velocity on temperature at low to moderate temperatures can be fit to an equation of the Arrhenius type only if a pre-exponential function of temperature and stress is incorpor-

ated. This pre-exponential function has nothing to do with the "entropy of activation", which is assumed zero; it is rather associated with dislocation activation across barriers having a distribution of effective strengths. The pre-exponential function approaches a constant as temperature approaches zero.

Before documenting these results we briefly review the governing equations of this problem and the nature of our computer code.

## 2. COMPUTER PROGRAM AND PERTINENT EQUATIONS

The computer program generates a large number of randomly distributed point barriers in a square area representing the slip plane. In general we used 999 point arrays but 500 point arrays were used to check results. Barriers on either side of this square area are considered to be in mirror image positions with respect to the side boundaries. This boundary condition physically approximates a free surface or grain boundary.

An initially straight dislocation of constant line energy is introduced at the bottom of the array. A shear stress,  $\tau$ , is applied to the dislocation in the direction of the Burgers vector. The dislocation moves forward bowing between obstacles to an equilibrium radius of curvature,  $R^*$ , given in dimensionless form by

$$R^* = R/L_s = \Gamma/\tau L_s b = 1/2\tau^* \quad [1]$$

where

$$L_s = \sqrt{A_p} \quad [2]$$

and

$$\tau^* = \tau L_s b / 2\Gamma \quad [3]$$

In this equation  $A_p$  is the mean area per obstacle,  $\Gamma$  is the line tension,  $b$  is the Burgers vector, and  $\tau$  is the applied stress.

If the dimensionless applied stress  $\tau^*$  is less than the zero degree yield stress,  $\tau_y^*$ , the dislocation will be stopped somewhere in the array. In our computer code the stable configurations are found using a circle rolling algorithm. The dislocation line will be arrested by an obstacle if the force on the obstacle is less than the obstacle strength. The force on obstacle  $i$  is given by  $2\Gamma \cos(\psi_i/2)$ . The obstacle strength is  $2\Gamma \cos(\psi_c/2)$ . Hence the condition for obstacle  $i$  to stop the dislocation is

$$2\Gamma \cos(\psi_i/2) < 2\Gamma \cos(\psi_c/2) \quad [4]$$

or

$$\psi_i > \psi_c$$

This condition is illustrated in Fig. 1. When the condition [4] is obeyed for all obstacles on the dislocation line the line will be arrested, giving a mechanically stable position. If no mechanically stable positions can be found, the stress is equal to or higher than  $\tau_y^*$ . Foreman and Makin<sup>3</sup> determined  $\tau_y^*$  values as a function of  $\psi_c$  using a similar computer experiment.

At a finite temperature a dislocation can move by thermally activating past barrier obstacles. This facility is included in our numerical code. In its most general form<sup>2</sup> the code computes the stochastic probability for activation past each of the obstacles against which the dislocation is pressed and forms an appropriate product of these to obtain the stochastic probability of activation past the line configuration of

obstacles. The code then calls two random numbers. The first is used to determine the time required for the dislocation to activate. The second is used to identify the particular obstacle which is cut. The code cuts this obstacle and searches the array until a new stable configuration of obstacles is found. In this code the activation trials are independent events; the dislocation does not remember past failures. The sequence of stable dislocation configurations taken on is, however, Markovian; the probability that a dislocation will be found in a certain configuration is a function of the previous configuration only. The velocity is computed as the reciprocal of the time ( $t$ ) necessary for the dislocation to sweep through the array. In dimensionless form:

$$v^* = \frac{L}{L_s vt} \quad [5]$$

where  $v^*$  is the dimensionless velocity,  $v$  is the attempt frequency (assumed constant), and  $L$  is the edge length of the square array.

Using the statistics of the activation process and approximations identified in the course of this work<sup>1, 2</sup> we have devised simplifications of the general code which allow rapid approximate treatment of dislocation behavior over a range of conditions. A particularly useful procedure, valid at low temperature, is the "minimum angle" approximation. As temperature is lowered it becomes increasingly likely that the dislocation will cut a line of barrier obstacles at the weakest point, that is, that it will activate past the particular obstacle at which the angle  $\psi$  takes on its minimum value. Since the expected value of the time,  $\langle t \rangle$ , to transit the array is just the sum of the expected times,  $\langle t_i \rangle$ , to activate past each of the stable configurations

in the array, we obtain a good low-temperature approximation with a code which activates the dislocation past each configuration by breaking the "minimum angle" in the expected time  $\langle t_i \rangle$ .

This approximation greatly simplifies the numerical analysis. The sequence of obstacle configurations encountered as a dislocation moves through an array in the "minimum angle" mode is a function of the applied stress only. The stability of a given line depends on the stress and on the obstacle strength, but is independent of temperature. Temperature enters the problem only in the computation of expected activation times.

In order to determine the expected activation time  $\langle t_i \rangle$ , for a line having minimum angle  $\psi_{\min}$ , we must compute the activation energy  $G_{\min}$ . To do this we assume an obstacle-dislocation interaction function,  $F(x)$ . Fig. 2a shows a general dislocation-obstacle interaction. Assuming that  $F$  increases monotonically to  $F_{\max}$ , the activation energy,  $G_{\min}$ , is given by

$$G_{\min} = 2\Gamma d [F(\beta_c) - F(\beta_i)] \quad [6]$$

where  $d$  is the characteristic width of the obstacle,  $\beta_i = \cos \psi_{\min}/2$  and  $\beta_c = \cos \psi_c/2$ . For our initial studies we selected a simple rectangular dislocation-obstacle interaction shown in Fig. 2b. In this special case equation [6] reduces to

$$G_{\min} = 2\Gamma d (\beta_c - \beta_i) \quad [7]$$

The average waiting time for a dislocation is then given by

$$\langle t_i \rangle = \exp \alpha (\beta_c - \beta_i) \quad [8]$$

with



$$\alpha = \frac{2\tau^*d}{kT} \quad [9]$$

The parameter  $\alpha$  is a dimensionless reciprocal temperature. It has a physically realistic minimum of  $\sim 10$ . It lies in the range  $10^2 - 10^4$  for typical metals at room temperature, and increases without bound as temperature approaches zero.

### 3. CHARACTERISTICS OF DISLOCATION MOTION

The points we wish to emphasize in this paper are most easily discussed in the "minimum angle" approximation, which we have found<sup>2</sup> to be qualitatively accurate and numerically reasonable for  $\alpha \geq 100$ . As the dislocation moves through the array, in this approximation, it encounters a sequence of lines uniquely determined by the applied stress. Each of these lines has a "strength"  $\beta_i$  which is also uniquely determined by the stress. A typical normalized distribution of  $\beta_i$  values is shown in Fig. 3; this is a composite distribution found by compiling the strengths of all lines encountered in passage through twenty 999 point arrays at two stresses:  $\tau^* = 0.1$  and  $\tau^* = 0.3$ . Given an obstacle strength,  $\beta_c$ , all lines having  $\beta_i \leq \beta_c$  will arrest the dislocation and must be passed thermally; lines having  $\beta_i > \beta_c$  will be mechanically cut. The yield strength of the array at obstacle strength  $\beta_c$  is that stress just sufficient to cause all lines to have  $\beta_i \geq \beta_c$ ; at  $\tau_y^*$ ,  $\beta_c = \beta_0$ , where  $\beta_0$  is the strength of the strongest line encountered. The expected waiting time  $\langle t_i \rangle$  at a line of strength  $\beta_i < \beta_c$  is given by equation [9]. The expected time to transit a given array is the sum of  $\langle t_i \rangle$  over all stable lines encountered.

(a) Jerky glide

Except under conditions of very low  $\alpha$  or very low  $\beta_c$  the motion of a dislocation through a random array of obstacles is jerky. A plot of the area swept out versus time is stepped, reflecting a tendency of the dislocation to glide quickly (relative to the total transit time) from one strong configuration to another. The phenomenon is illustrated in Figs. 4 and 5. Fig. 4 (a-d) shows the effect of temperature at constant stress. The jerkiness of the motion increases strikingly and monotonically as  $\alpha$  is raised. Fig. 5 (a-d) shows the effect of stress at constant temperature. The motion tends to be more jerky at high stress, but the effect is less pronounced. In fact, increasing the stress from  $\tau^*/\tau_y = 0.4$  to  $\tau^*/\tau_y = 0.6$  resulted in a slightly smoother glide through this particular array.

The reason for "thermal jerkiness" is straightforward. Compare the relative waiting times of two lines of differing strength, say  $\beta_1 < \beta_2$ . By equation [8]

$$\langle t_1 \rangle / \langle t_2 \rangle = \exp \alpha [\beta_2 - \beta_1]. \quad [10]$$

The ratio of expected activation times increases exponentially with  $\alpha$ ; given that the dislocation encounters obstacle configurations having a distribution of  $\beta$  values the flow necessarily becomes more jerky as  $\alpha$  is raised. As temperature approaches zero  $\alpha$  increases without bound, and an area-time profile approaches a simple step shape with the dislocation spending virtually its whole transit time in the strongest configuration ( $\beta_0$ ). Since the difference  $\beta_1 - \beta_2$  cannot exceed  $\beta_c$ , "thermal jerkiness" is less noticeable when the obstacle strength is very small.

The source of the "mechanical jerkiness" illustrated in Fig. 5 is more subtle. Raising the applied stress ( $\tau^*$ ) affects the dislocation motion in two ways. First, as may be seen in Fig. 3, the distribution of line strengths is changed. The value ( $\beta_0$ ) of the strength of the strongest line encountered is raised by an amount which, for  $\tau^* \lesssim 0.5$ , is given approximately by the Friedel relation,<sup>2-4</sup>

$$\beta_0 \propto (\tau^*)^{2/3}. \quad [11]$$

At the same time the shape of the distribution is changed. The distribution is broadened to spread over a larger range of  $\beta$  values. There tend to be fewer lines having  $\beta$  near  $\beta_0$  at higher stress. The second effect is a change in the fraction of unstable lines. This fraction increases with the stress. More lines are mechanically cut at higher stress; fewer must be passed thermally.

We may easily show that the first rather than the second of these effects is principally responsible for "mechanical jerkiness". The velocity of the dislocation is largely determined by those lines whose expected waiting times are within an order of magnitude of the expected time to activate past the strongest line in the array. By equation [8], such lines have  $\beta_i$  values

$$\beta_i < \beta_0 + \frac{2.3}{\alpha} \quad [12]$$

The mechanical cutting of lines will have an important effect on velocity only if lines of this strength can be cut, i.e., if  $\beta_c$  satisfies the inequality [12]. Using the Friedel relation [11] we obtain the condition

$$1 - (\beta_0/\beta_c) = 1 - (\tau^*/\tau_y^*)^{2/3} < \frac{2.3}{\alpha\beta_c} \quad [13]$$

for mechanical cutting to have an important effect on the "jerkiness" of the motion. The inequality [13] will be satisfied only if the applied stress is high ( $\tau^*$  near  $\tau_y^*$ ) or if  $\alpha$  or  $\beta_c$  is small. When  $\alpha = 100$  and  $(\tau^*/\tau_y^*) = 0.8$  mechanical cutting can be neglected if  $\beta_c > \frac{1}{6}$  or  $\psi_c < 161^\circ$ .

On the other hand, the tendency of the stress to broaden the distribution of line strengths has the consequence that the number of lines which satisfy the inequality [12] tends to decrease as the stress is raised, hence increasing the "jerkiness" of the flow. However, while the effect of increasing temperature is mathematically certain, the effect of increasing the applied stress is only statistically likely; one will occasionally find that raising the stress causes smoother dislocation glide through a particular array, as illustrated in the example of Fig. 5.

(b) The velocity-temperature relation

Fig. 6 shows the relation between dislocation velocity and dimensionless reciprocal temperature for several values of the applied stress for a given 999 point array of fixed obstacle strength. The data were computed with our code operating in the "minimum angle" mode. The curves giving  $(- \ln v^*)$  as a function of  $\alpha$  bend upward; they may be fit by equations of the Arrhenius form only if pre-exponential functions of  $\alpha$  are incorporated. The concavity of these curves is again due to the fact that the dislocation encounters lines having a distribution of strengths as it moves through the array.

The velocity  $v^*$  is proportional to the inverse of the time spent in traversing the array (equation [5]). If  $n + 1$  stable obstacle configurations are encountered, numbered  $0, \dots, n$  in order of increasing strength, and if each is assumed to be thermally passed in its expected time, then

$$v^* = C \left( \sum_{i=0}^n \langle t_i \rangle \right)^{-1} = CS^{-1} \langle t_0 \rangle^{-1} \quad [14]$$

where  $C$  is a constant,

$$S = 1 + \sum_{i=1}^n \langle t_i \rangle / \langle t_0 \rangle \quad [15]$$

and  $\langle t_0 \rangle$  is the activation time for the strongest line in the array.

Using equation [8],

$$-\ln v^* = \ln S + \alpha [\beta_c - \beta_0] + \ln C, \quad [16]$$

which is of the Arrhenius form with pre-exponential function  $S$ . From equation [11]  $S$  is seen to be a function of  $\alpha$  and  $\tau^*$ . It approaches 1 as  $\alpha$  becomes very large ( $T$  approaches zero). Equations [11] and [12] show that  $S$  is a monotonically decreasing function of  $\alpha$ , hence the concavity of the curves in Fig. 6.

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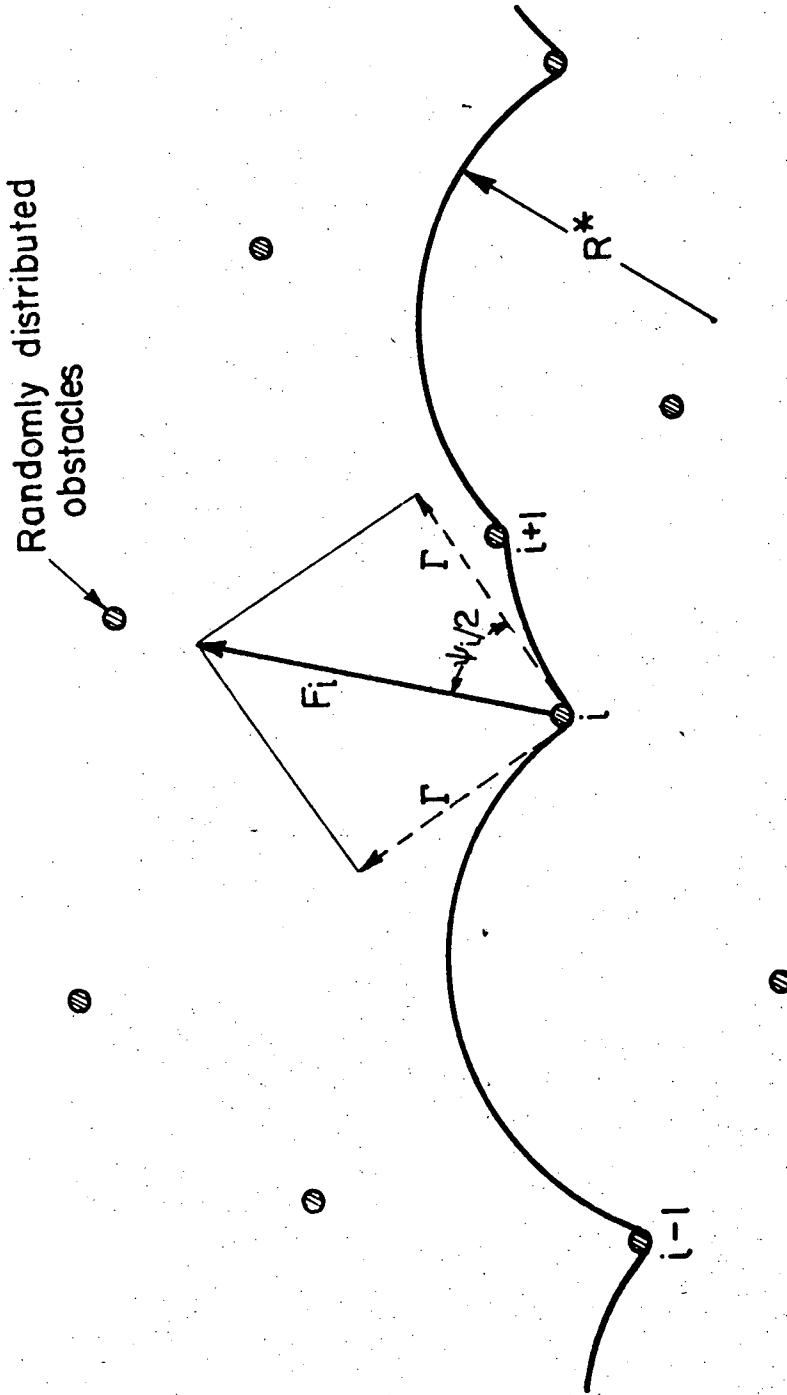
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Chapter VIII.

FIGURE CAPTIONS

- Fig. 1. Configuration of a dislocation pressed against an array of obstacles by a stress  $\tau$ .
- Fig. 2. Possible force displacement relations for dislocation obstacle interaction in the limit of small obstacle size. The relation illustrated in (b) was used in the computations reported here.
- Fig. 3. Distribution of line strengths encountered in dislocation passage through 20 distinct 999 point arrays at two stresses: (a)  $\tau^* = 0.1$ , (b)  $\tau^* = 0.3$ .
- Fig. 4. The effect of temperature on the jerkiness of dislocation glide. The area swept out by the dislocation is plotted against dimensionless time ( $t^* = vt$ ) at four values of dimensionless reciprocal temperature  $\alpha$ . In these runs  $\tau^* = 0.4, \beta_c = 0.63$ .
- Fig. 5. The effect of stress on the jerkiness of glide. The area swept out by the dislocation is plotted against dimensionless time at four values of the parameter  $\tau^*/\tau_y^*$ . In these runs  $\alpha = 100$ ;  $\beta_c = 0.63$ .
- Fig. 6. The effect of temperature on velocity. Note the upward concavity of the curves.

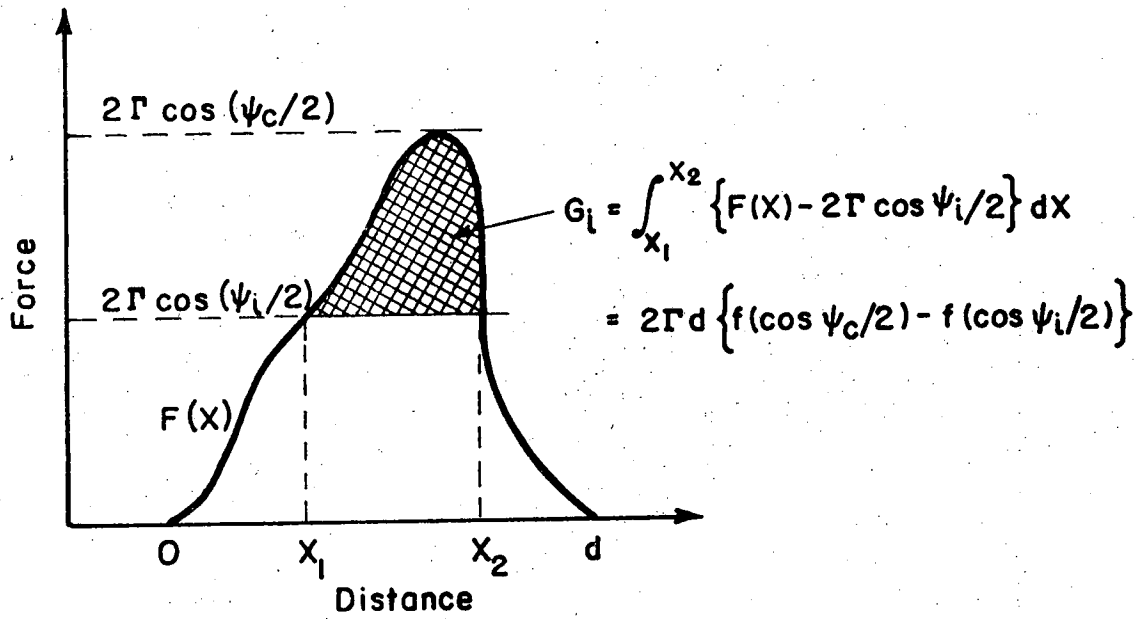




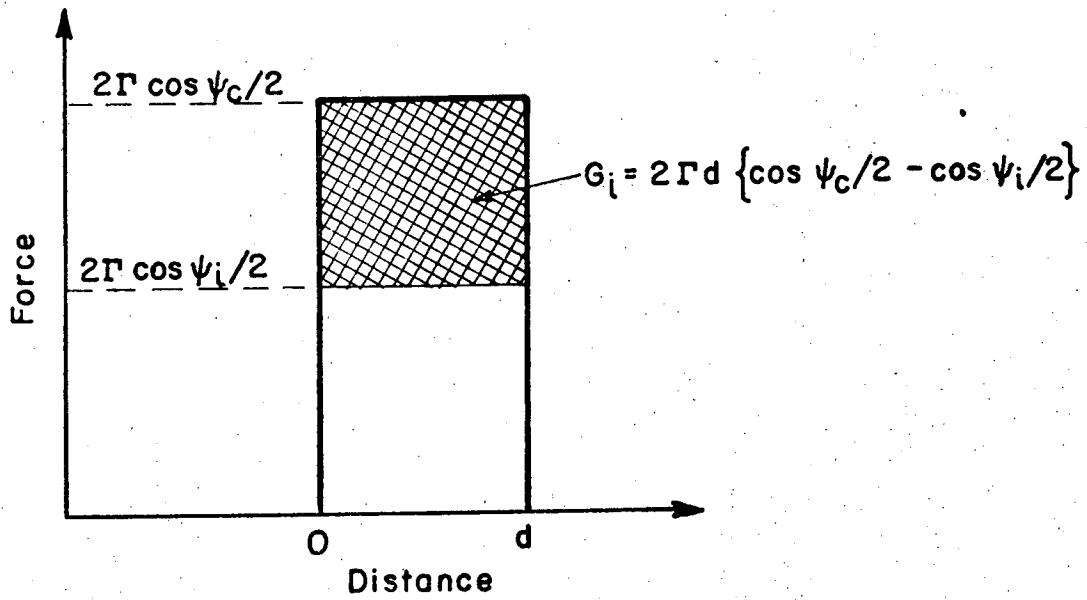
$$F_i = 2\Gamma \cos(\psi/2)$$
$$R^* = 2R/L_s = 1/\tau^* = \frac{2\Gamma}{\tau L_s b}$$

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Fig. 1.



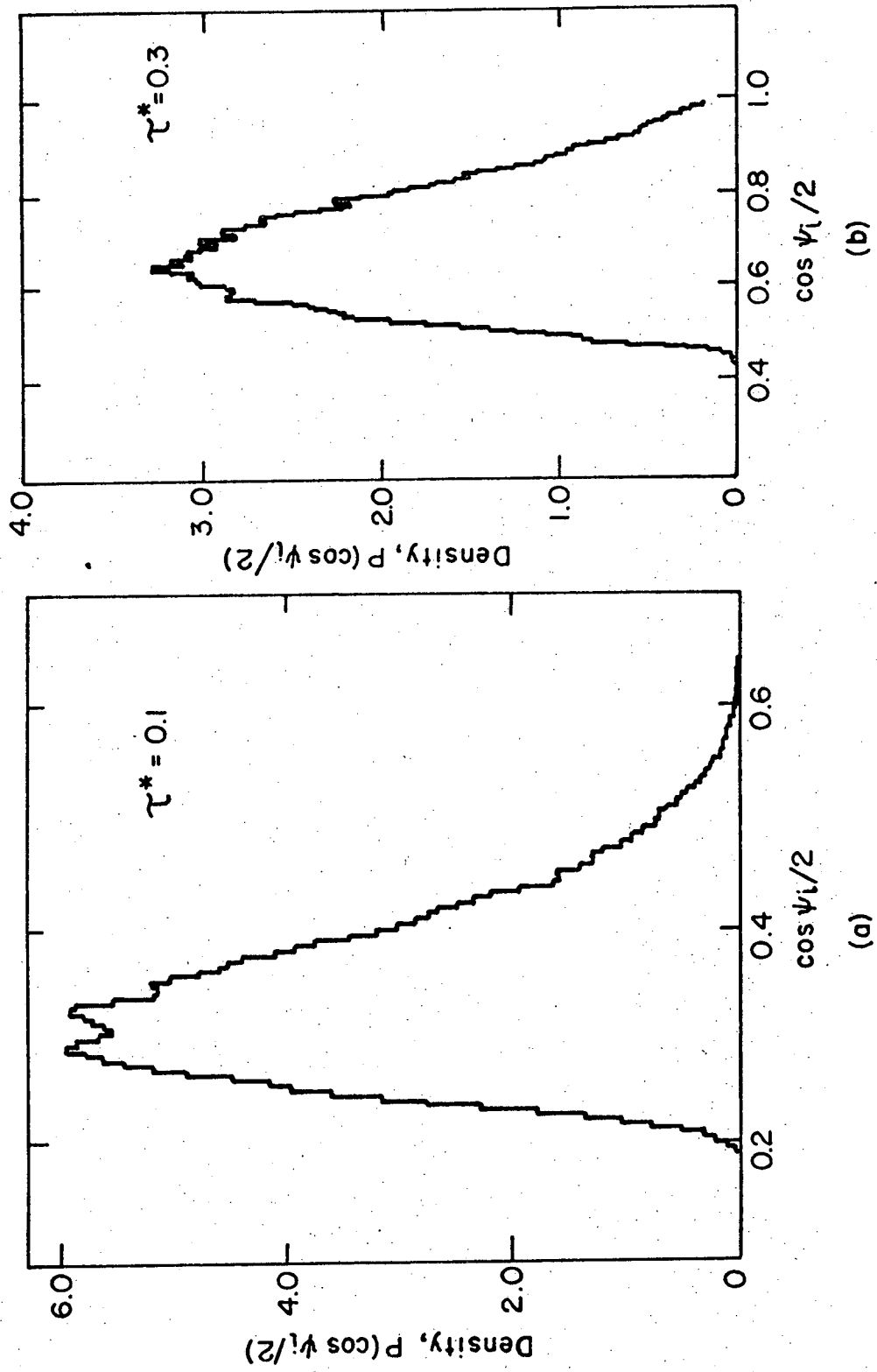
(a)



(b)

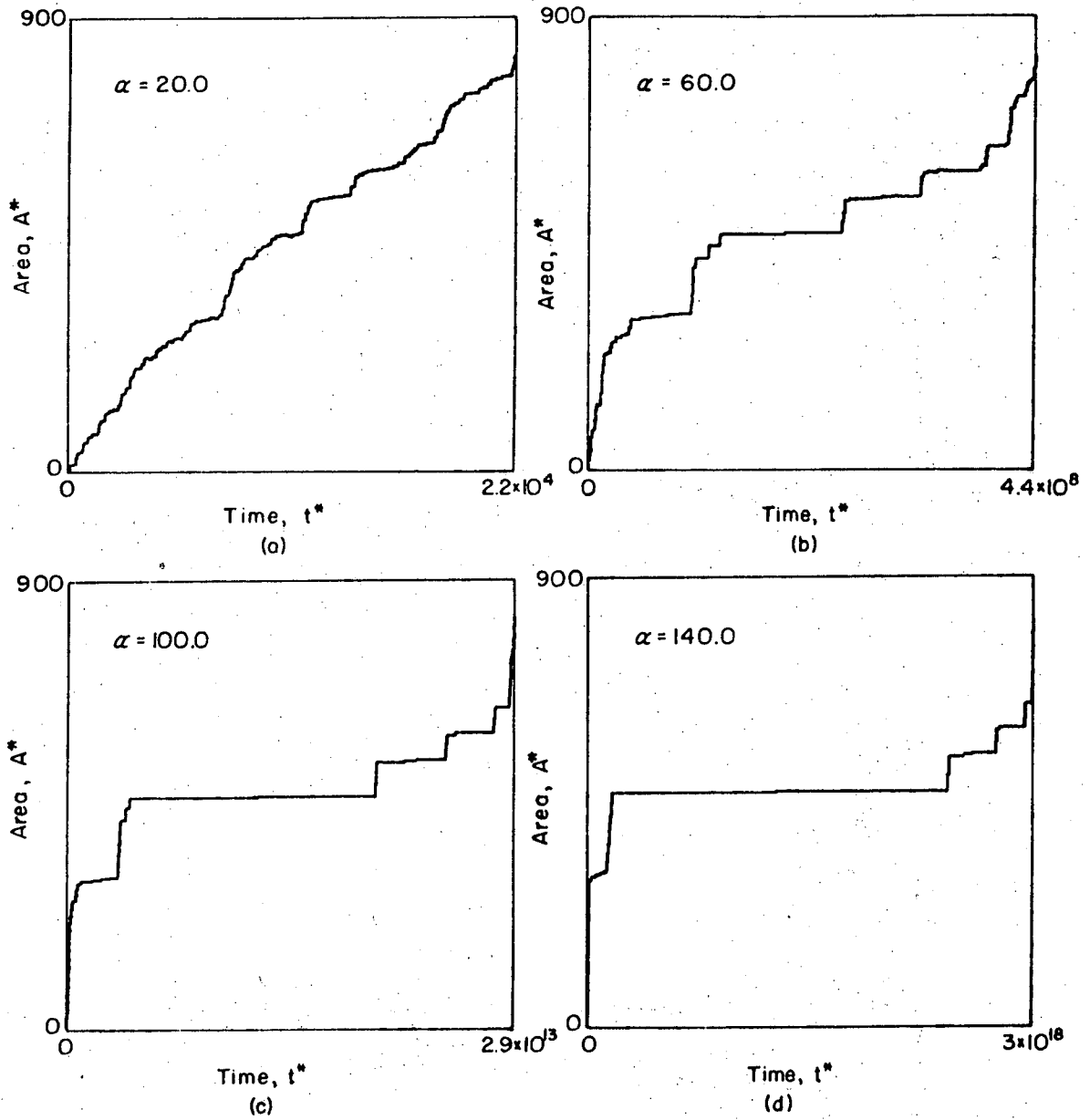
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Fig. 2.



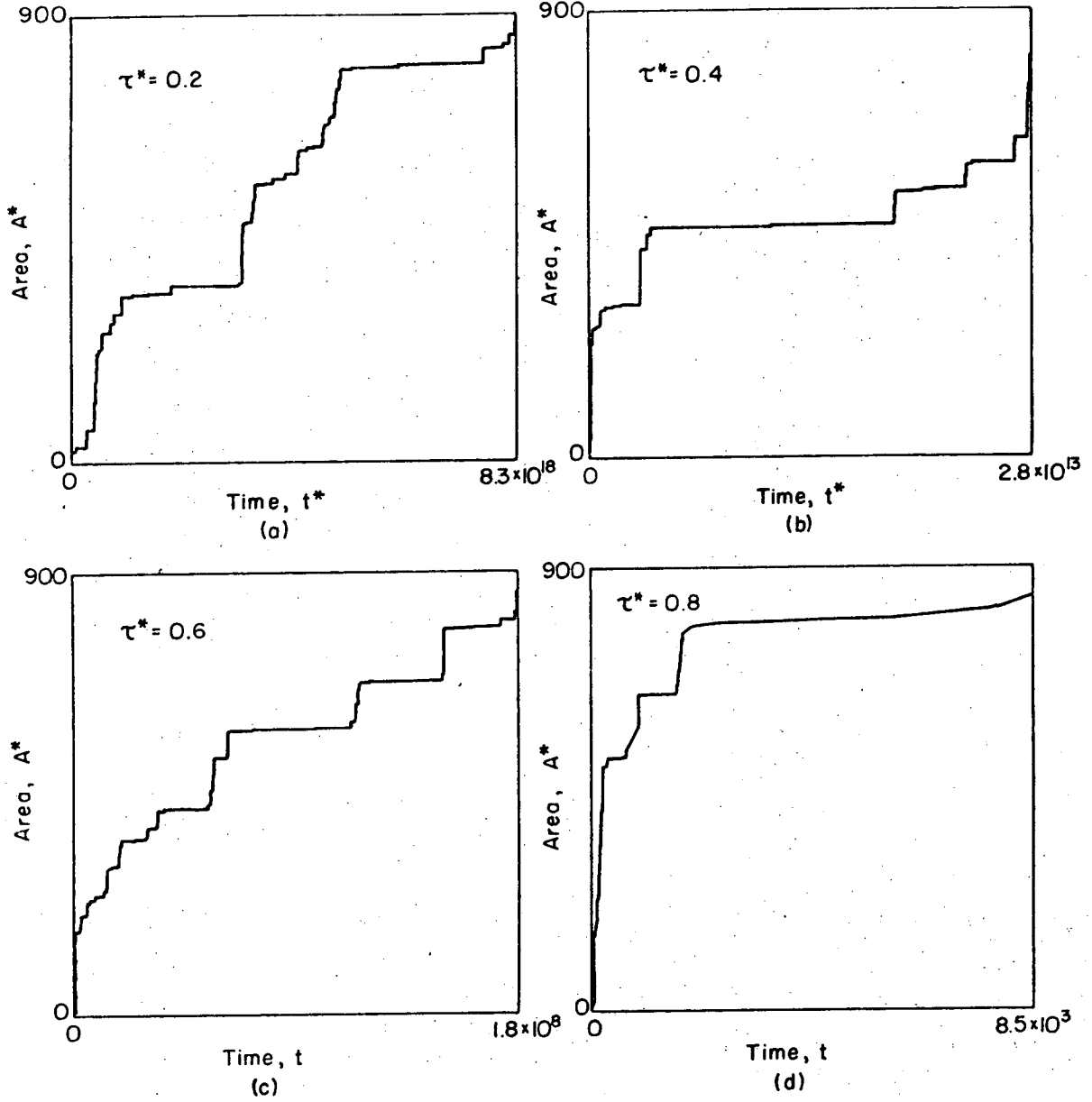
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Fig. 3.



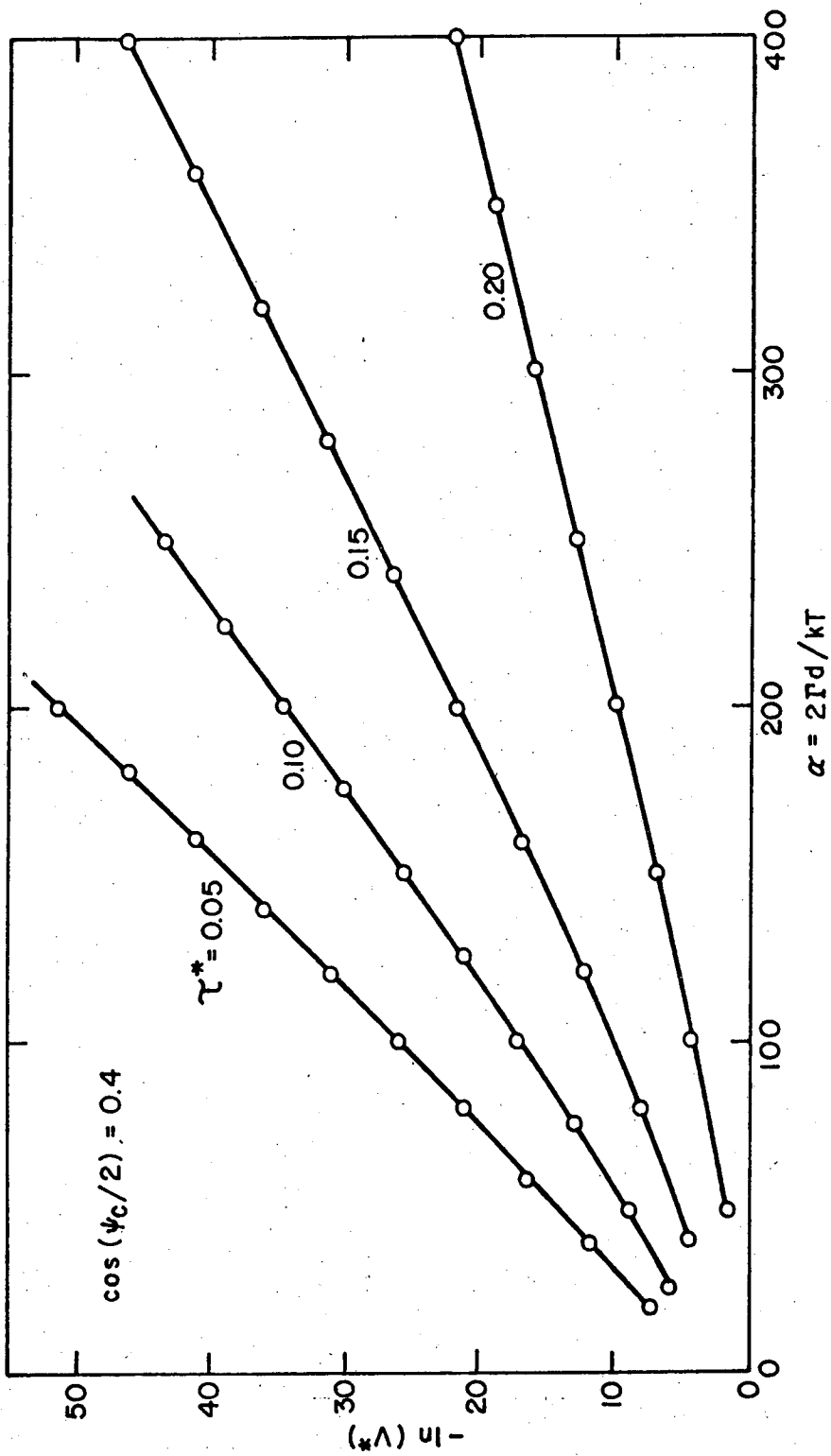
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Fig. 4.



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Fig. 5.



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Fig. 6.

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