Computer Simulation of Solid Solution Strengthening in Fcc Alloys: Part I. Friedel and Mott Limits

R.J. ARSENAULT, S. PATU, and D.M. ESTERLING

It has been assumed for a number of years that dilute solid solutions obey a Friedel limit; *i.e.*, the concentration dependence of the yield stress varies as 1/2 power ($c^{1/2}$), whereas in more concentrated solid solutions, the Mott limit is upheld with a predicted concentration dependence of $c^{2/3}$. These two limits were examined both analytically and numerically. As expected, the Friedel limit can be reproduced without any difficulty. However, in the Mott limit, a detailed analytical treatment of the concentrated solution case resulted in a concentration dependence of the yield stress as $c^{1/2}$. The numerical data are in agreement with this analytical result in the Mott limit. Earlier work which predicted a $c^{2/3}$ dependence is analyzed, and certain key assumptions are shown to be invalid.

I. INTRODUCTION

THEORIES of solid solution strengthening in fcc solids have proceeded using analytical models[1–21] and computer simulation models.[22–27] The analytical models often provide useful qualitative and, in some cases, quantitative insights into solid solution effects. However, in order to make the analytical models tractable, often somewhat arbitrary assumptions are introduced into the treatments. Computer simulation techniques afford the opportunity to solve for the behavior of a model over a wide range of parameters (such as concentration, obstacle strength, or dislocation line tension), with the only restriction being the numerical accuracy of the particular computer configuration or program.

Two important limits may be identified in solid solution strengthening: the low concentration, high obstacle strength limit, or the Friedel limit, and the high concentration, low obstacle strength limit, or Mott limit.[20] In this investigation, we will summarize some of the assumptions made in evaluating the yield stress behavior in these limits, particularly the Mott limit, and compare the results of some analytical models with our computer simulation. Not surprisingly, we will reproduce the key analytical result in the Friedel limit, namely, that the yield stress varies as the square root of concentration. However, we will report that this same square root of concentration dependence is also valid in the Mott limit. This is at variance with the concentration to the 2/3 power derived by a number of authors for the Mott limit.[8,9,16,17,20] We will point out certain questionable assumptions made in these studies and further point out that our results are in agreement with the results of Kuo and Arsenault[27] in the extreme Mott limit of a straight dislocation line (*i.e.*, infinite line tension).

This paper concerns itself with establishing the behavior of our numerical model in these important limits and contrasts our results, particularly the concentration dependence, with those derived from analytical models. The succeeding paper will provide details of the simulation method and will derive the general dependence of the yield stress on line tension and obstacle strength as well as concentration. Section II provides some background on earlier work. Section III contains an analytical treatment of the Mott limit, showing the need to take special care of fluctuations in the restoring forces. Section IV summarizes the simulation method used to generate the numerical results in Section V.

R.J. ARSENAULT, Professor and Director, and S. PATU, Visiting Scholar from the Institute of Metals Research, Academica Sinica, Shenyang, The People's Republic of China, Research Associate, are with the Metallurgical Materials Laboratory, University of Maryland, College Park, MD 20742-2111. D.M. ESTERLING, Professor, is with the Civil, Mechanical, and Environmental Engineering Department, George Washington University, Washington, DC 20052.

Manuscript submitted January 20, 1988.

II. FRIEDEL AND MOTT STATISTICS

We will refer to the results of the analytical theories in their respective limits as Friedel and Mott statistics. In the Friedel model, the obstacles are assumed to be discrete, *i.e.*, nonoverlapping, and the dislocation encounters and overcomes a single obstacle in its motion forward. The strength of one obstacle is proportional to a parameter f. The dislocation is assigned a line tension (Γ), and under an applied stress, the dislocation bows out, moves between, and overcomes certain obstacles. In the steady state, a dislocation released at one obstacle moves forward and encounters exactly one more obstacle.[20] With these assumptions, the yield stress across the slip plane becomes

$$\tau_{\text{FRIEDEL}} = f^{3/2}\left(\frac{2\Gamma}{\mathbf{b}l}\right) \qquad [1]$$

where Γ is the line tension, $\mathbf{b}$ is the Burgers vector for the dislocation, and l is the average interobstacle spacing. In the low concentration limit, l is inversely proportional to the square root of the concentration and the combined concentration (c), line tension, and obstacle strength dependence of the yield stress for Friedel statistics[20] are

$$\tau_{\text{FRIEDEL}} = k\Gamma f^{3/2} c^{1/2} \qquad [2]$$

where k is a constant depending upon the obstacle geometry. We confine ourselves to lowest order terms in the concentration (assuming, as appropriate for the Friedel limit, that $c \ll 1$).

Although the derivation of the Friedel statistics is straightforward, there are at least two issues which should be considered. If we are considering solid solutions, it is not obvious how one would obtain a specific value of the yield stress. This uncertainty is related to the parameters k and f, which are ill-defined. Is every solute atom an obstacle? Are only pairs of solute atoms to be considered obstacles? How is f related to the solute atom-dislocation interaction? None of these questions is addressed explicitly in the generic derivation of Friedel statistics. Their answer requires a detailed solution (such as that provided in this paper). The second issue is related to the upper limit of concentration for the Friedel limit. If we consider the upper limit of Friedel statistics, as proposed by Nabarro:[16]

$$\frac{c}{f}\left(\frac{w}{\mathbf{b}}\right)^2 = 1 \qquad [2a]$$

where w is the width or effective range of interaction of the obstacle and the dislocation line,[20] and we use Kocks *et al.*'s estimates[20] for the width, w, and obstacle strength, f, then for a yield stress $\tau = 10^{-4}\,\mu$, the upper limit for the concentration to be in the Friedel limit is $c \approx 5 \times 10^{-3}$. Labusch (see Reference 20) suggests that the right-hand side of Eq. [2a] is 1/36. This gives an upper limit in concentration of $c \approx 10^{-4}$. Therefore, there is a significant difference in the estimated upper limit concentration of the Friedel statistics.

Kocks *et al.*[20] also provide a succinct derivation of Mott statistics. In the Mott limit, the obstacle strength is small and the concentration is higher (c ranges from 0.01 to 0.10). In this limit, it is commonly assumed that the dislocation line is almost straight, as in the derivation in Reference 20, where the excursion in the dislocation line shape over an appropriately long segment of the dislocation line is taken to be the width of a dislocation obstacle. This derivation produces the following relation, which we will refer to as Mott statistics:

$$\tau_{\text{MOTT}} = \mu(\bar{f})^{4/3} c^{2/3} \left(\frac{w}{\mathbf{b}}\right)^{1/3} \qquad [3]$$

Here μ is the shear modulus, c is the concentration, $\mathbf{b}$ is the Burgers vector, w is the obstacle width (presumably, the interaction of a single solute atom and the dislocation line), and $\bar{f}$ is—in the words of Kocks *et al.*—"a somewhat vaguely defined average obstacle strength." In addition, this derivation involves a parameter n: the number of random bends in the dislocation line over a length of the dislocation line that yields a net bend of width w. We view the parameter n as also somewhat "vaguely defined."

A problem with this derivation is that various uncertain assumptions are made, in particular involving the relation of the parameter n to the other model parameters. Little, if any, justification is provided. Yet, the derivation in Reference 20 shows that the parameter n ends up controlling the concentration dependence in Eq. [3]. Our numerical results in the Mott limit will demonstrate that a $c^{1/2}$ power law is to be preferred over a $c^{2/3}$ power law—demonstrating a concern for the above assumptions. More will be said concerning this and related derivations in the next section.

Labusch[8] also proposed a $c^{2/3}$ dependence of the yield stress in the Mott limit. His analysis was based on a statistical theory, with a key assumption that the distribution of obstacles along the dislocation line varies slowly compared with the variation in the force relation between the dislocation line and a single obstacle. This condition is formalized in a later paper[28] as requiring that the parameter:

$$\rho_o = c^{1/2}\left(\frac{w}{\mathbf{b}}\right)\left(\frac{f_o}{2\Gamma}\right) \qquad [4]$$

be small. Here, f_o is the obstacle strength (presumably, the interaction of a single atom and the dislocation line), and Γ is the line tension. The claim is that so long as ρ_o is small, the solution is correct. However, we will present a pseudorandom model in the next section which obeys this constraint, which is trivially soluble and which produces a $c^{1/2}$ dependence in the yield stress in the Mott limit. The problem—as will be emphasized in the next section—is the equating of the average force per unit length on the dislocation line to the applied force per dislocation line length ($\tau_c \mathbf{b}$) to arrive at the critical stresses τ_c. In the extreme Mott limit (large line tensions), the average force vanishes, but *fluctuations* in the force on the dislocation line remain substantial. As we have emphasized in an earlier paper,[19] it is these fluctuations, not some average force, which control the yield stress in the Mott limit.

Schwartz and Labusch[28] have presented a numerical solution of the Labusch statistical treatment. The condition for the critical stress is different from the earlier treatment in that with the obstacles (it is not specified in Reference 28 whether this is a single solute atom or a special configuration of solute atoms) placed on the slip plane according to a Poisson distribution, the applied stress is increased incrementally in a (revised) force balance equation until the dislocation achieves unbounded motion. Schwartz and Labusch obtained a best fit of $c^{2/3}$ in the concentration dependence of the critical stress. As with any numerical solution, there are uncertainties in interpretation. The solution was obtained on a lattice of 30 by 30 "normalized units" (*i.e.*, 900 obstacles) over a grid which apparently has 750 by 30 elements, with periodic boundary conditions applied on the glide direction and in the dislocation line direction. Schwartz and Labusch[28] replaced the actual obstacles by infinitely narrow obstacles on a transformed lattice. Hence, we cannot establish a one-to-one comparison between our numerical solution (based on actual obstacles in physical space) and their numerical solution. However, we did find that our numerical solution very definitely depended upon the size of the lattice containing the randomly placed solute atoms. The large scatter in their data (Figure 5 of Reference 28) is to be noted in the Mott limit. This scatter might be reduced with a larger random system.

Nabarro[18] has provided a derivation of the concentration dependence of the yield stress in the Mott limit and also obtained $c^{2/3}$ behavior. As in the earlier Labusch paper, Nabarro focused on the *average* restoring force

due to the random obstacles acting on a unit length of dislocation when it moves a unit displacement from its equilibrium position. It has been shown[19] that even when the *average* restoring force on a unit length of dislocation is zero, the fluctuation of this restoring force is not zero. If the limiting case of a rigid dislocation line is considered, then Nabarro predicts (Eq. [22], Reference 18) that the average restoring force should be zero and concludes that the yield stress vanishes in the rigid dislocation (infinite Γ) limit. It has been shown[19,27] that the average value of the restoring force is zero if the average is taken over *all* positions of the dislocations on the slip plane, as it should be. However, for any given position, there can be a large restoring force on a unit length of dislocation line. As shown in Reference 27, the maximum restoring force on a straight dislocation scales as inversely proportional to the square root of the dislocation line length. The numerical results of Reference 27 generated a yield stress that varied between 10 and 100 pct of the experimentally expected yield stress at absolute zero as the line length varied between 10^{-2} and 10^{-4} cm. These later lengths are typical distances between pinning points (*e.g.*, grain and subgrain boundaries) in most test specimens. Unfortunately, Nabarro does not properly account for the fluctuations in this restoring force that dominate the critical stress in the Mott limit. In the next section, we address the issue of fluctuations in more detail.

III. MOTT LIMIT ANALYSIS

Kuo and Arsenault[27] have provided a detailed numerical analysis of the movement of a straight dislocation in a concentrated solid solution. This is the extreme Mott limit of infinitely large line tension. They obtained a critical stress as:

$$\tau_c = \frac{F_o}{\mathbf{b}L^{1/2}} \qquad [5]$$

where F_o is proportional to $[c(1 - c)]^{1/2}$ over a very wide concentration range, and L is the length of the straight dislocation line segment. Even though their scatter was very small, it may be argued that this is still a numerical result and subject to some variance. Hence, we now present two models, which obey the key assumption made in initiating the Labusch statistical treatment (ρ_o, is small, Eq. [4]) and which also generate a $c^{1/2}$ dependence in the critical stress, which are trivially soluble in the Mott limit.

The two models are (I) a regular array of obstacles, with spacing l and (II) an array of obstacles which are randomly placed, on average, a distance l apart, along straight lines with each line parallel and regularly spaced a distance l apart. In the Mott limit (large line tension, small obstacle strength), the dislocation is treated as a straight entity. A dislocation line of length L experiences a maximum restoring force of $(L/l)f_o$ (each obstacle consists of a potential well with slope f_o) when aligned along the parallel lines in model II or the regular arrays in model I. If the obstacles are placed on a three-dimensional lattice, with lattice spacing $\mathbf{b}$, then the concentration of obstacles on the slip plane is $c = \mathbf{b}^2/l^2$ for both models. For both models then, the critical stress τ_c is given by the relation:

$$\tau_c\mathbf{b} = \text{maximum restoring force per unit length}$$

$$= \left(\frac{f_o}{l}\right)\mathbf{b} = f_o c^{1/2} \qquad [6]$$

Note, for both models, that the restoring force—when averaged over the slip direction—is zero. (When the dislocation approaches a repulsive obstacle, it experiences a force f_o opposite to the direction of dislocation motion. As the dislocation passes the obstacle, it experiences a force f_o in the direction of motion.) This averaged restoring force also vanishes for a straight dislocation line in a fully random lattice. Note further that the Labusch parameter in Eq. [4] is small and indeed, vanishes. Here, we clearly see the failure of focusing on an average force and ignoring fluctuations in the restoring forces.

We introduced these two models since we can follow an analysis of these models using the statistical treatment of earlier authors. This immediately exposes the weakness of their approach, namely that fluctuations can be ignored and the yield stress can be equated to an average restoring force (as demonstrated by noting that their yield stress becomes zero in the infinite line tension limit). Now, it might be argued that these models still are quite regular. Perhaps there is some subtle effect in going to a fully random model. To the contrary, as we now espouse, the consideration of fluctuations is even more crucial in a fully random model.

In our two models, every obstacle is a "hard spot," *i.e.*, contributes to the critical stress. In a fully random model, there is considerable cancellation among the force fields due to the individual obstacles.[29] The "hard spots"—the regions of large restoring forces—consist of very special obstacle geometry. They consist of one or more obstacles (solute atoms in the treatment given in the succeeding paper) lined up along the dislocation line and surrounded by vacant lattice sites. Such an array is more effective than a general arrangement of n obstacles over some small region since, in general, the individual force fields from the obstacles cancel, leaving a small net contribution to the restoring force.[29] In a fully random model, the critical stress is related inversely to the spacing between these hard spots. In contrast to our models I and II, there is no clear cut definition in a fully random model as to precisely what constitutes a hard spot. However, clearly they are related to *fluctuations* in the obstacle distribution and not to *averages* of the obstacle distribution.

We close this section by proposing a revised approach to a statistical theory. Labusch focuses on an average force as:

$$\langle F \rangle = \int \rho(x,y)F(x,y)\,dx\,dy \qquad [7]$$

Here, $\rho(x,y)$ is the obstacle distribution seen by the dislocation line, and $F(x,y)$ is the restoring force at (x,y) due to an individual obstacle. As Labusch points out, $\rho(x,y)$ becomes equal to c for a straight dislocation line

(or in the extreme Mott limit). This average force vanishes for a straight dislocation line leading to a vanishing critical stress *if* $\tau_c \mathbf{b}$ is proportional to $\langle F \rangle$. We argue that consideration should be given to the fluctuation average:

$$\Delta F \equiv (\langle F^2 \rangle - \langle F \rangle^2)^{1/2} \quad [8]$$

where

$$\langle F^2 \rangle = \int \rho(x,y) F^2(x,y)\, dx\, dy \quad [9]$$

If $\Delta F \ll \langle F \rangle$, then the average restoring force controls the critical stress. However, as is the case in the Mott limit, if $\Delta F \gg \langle F \rangle$, then ΔF controls the restoring force. In the latter case, it is fluctuations in the obstacle distribution which generate hard spots which, in turn, determine the critical stress. For a straight dislocation, $\rho = c$ and $\langle F \rangle = 0$, so that:

$$\Delta F = c^{1/2} [\int F^2(x,y)\, dx\, dy]^{1/2} \quad [10]$$

This again demonstrates the square root dependence of the critical stress on the concentration and that the critical stress does not vanish in the extreme Mott limit.

To sum up, the $c^{2/3}$ dependence in τ_c, obtained by Labusch by equating $\langle F \rangle$ to $\tau_c \mathbf{b}$, actually behaves as $c^{2/3}\Gamma^{-1/3}$.[18] The $c^{1/2}$ dependence obtained by Kuo and Arsenault (which accounted for fluctuations) is in the infinite Γ limit. In the infinite Γ limit, the only terms which remain (do not diverge or go to zero) behave as Γ^0 (the line tension of a straight dislocation). Hence, the yield stress derived by Kuo and Arsenault actually behaves as $c^{1/2}\Gamma^0$. The term "weak obstacle" can be viewed alternatively as referring to "large line tension" (see Eq. [14] or the Labusch parameter in Eq. [4]). Hence, we can assess the relative importance of the Labusch *vs* Kuo-Arsenault contributions in the Mott limit by investigating their large Γ behavior. For any given concentration c and for a sufficiently large Γ, the Labusch $c^{2/3}\Gamma^{-1/3}$ dependence will be dominated by the Kuo-Arsenault $c^{1/2}\Gamma^0$ term in the critical stress.

Finally, it should be pointed out that these analytical theories of the Mott statistics do not result in a specific value of the yield stress, since various key parameters (*e.g.*, obstacle strength) remain ill-defined without any direct relation to measurable quantities.

We close this section by noting the work of Nixon and Mitchell,[30] which has been referred to by Nabarro as "very careful" experiments.[18] The data was analyzed by Nixon and Mitchell using statistical methods. Over the entire concentration range from 2 to 13.2 at. pct, a best fit of data gave a concentration dependence of $c^{0.51}$.

IV. SIMULATION PROCEDURE

The details of the simulation procedure are provided in the following paper. In the procedure, a fcc lattice was generated, and substitutional solute atoms were randomly distributed with a concentration range from 0.1 to 10 pct. This paper will be confined to the interaction between an edge dislocation strain field and the strain field due to a solute atom size misfit—the dominant interaction in our model. The interaction force per unit length on this dislocation due to the i-th solute atom, at position z along the dislocation line, is:

$$f(i)_{\text{size}} = \int_{z-\mathbf{b}/2}^{z+\mathbf{b}/2} \sigma(i)_{\text{size}}\, dz \quad [11]$$

$$\sigma(i)_{\text{size}} = 6\mu\varepsilon r_o^3 xy[x^2 + y^2 + z^2]^{-5/2} \quad [12]$$

Here, μ is the shear modulus, r_o is the radius of the solvent atom, ε is the misfit strain due to the size difference between the solute and solvent atoms, and $\mathbf{b}$ is the Burgers vector. The dislocation line is originally oriented in a straight line parallel to the z axis, and the force is the component in the slip direction, which is taken to be parallel to the x axis. For the purpose of evaluating the force, the origin is placed at the site of each solute atom.

The net force on a dislocation line segment at position (x,z) in the slip plane is then:

$$F_s(x,z) = \sum_{i=1}^{N} f(i) \quad [13]$$

The interaction is cut off at an outer radius of $4\mathbf{b}$. A separate study by Kuo and Arsenault[27] indicated that over a number of random solute atom configurations, the total force on a given segment of the dislocation line was written at 10 pct of the asymptotic value (determined at a cutoff distance of $50\mathbf{b}$) when the interaction range was truncated to $4\mathbf{b}$. The reported results also exclude the nearest neighbor atoms, as discussed in the following paper. Basically, these short-range interactions were excluded due to our lack of confidence in the use of elastic limit results on such an atomic scale. However, as a check, simulations also were run which included nearest neighbor terms, with these results in agreement with our qualitative conclusions regarding the yield stress dependence. The magnitude of the yield stress increased, but the concentration dependence remained the same.

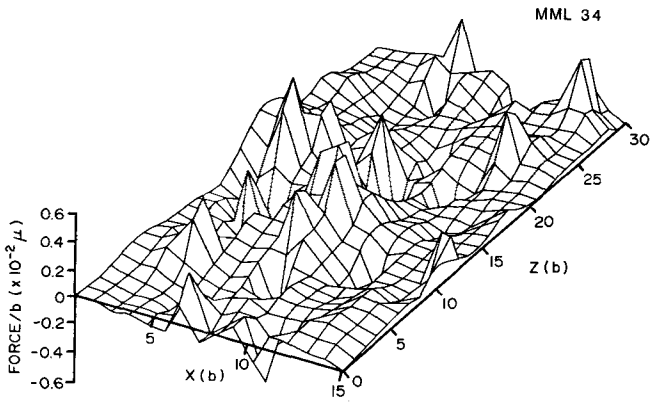
The force balance equation on each $1\mathbf{b}$ long segment of dislocation line is:

$$\Gamma \frac{d^2x}{dz^2} + \frac{F_s(x,z)}{\mathbf{b}} + \tau\mathbf{b} = 0 \quad [14]$$

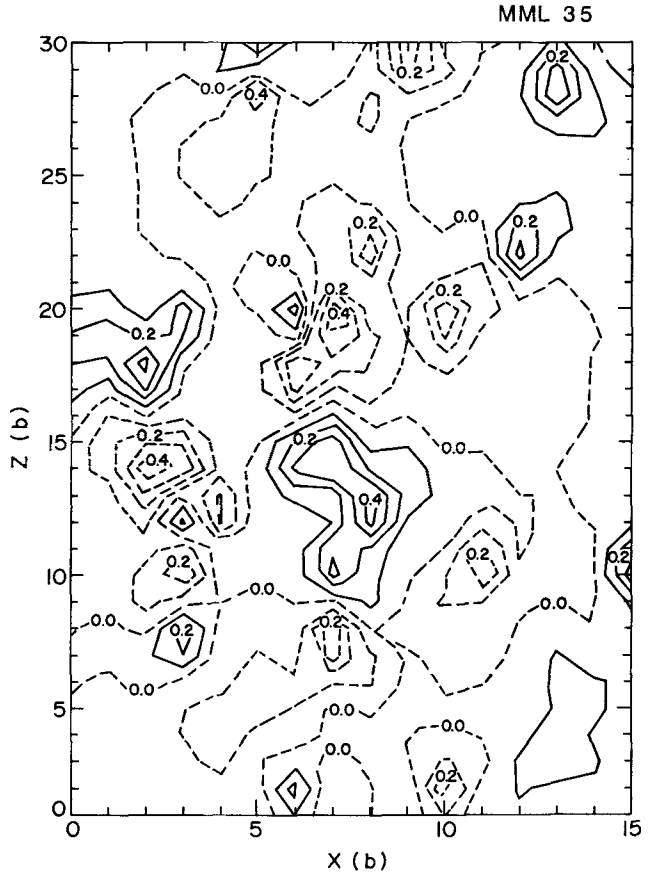
where τ is the externally applied shear stress. Unless explicitly stated otherwise, Γ was chosen as $0.5\ \mu\mathbf{b}^2$. (The Mott limit is obtained with a weak obstacle strength.) An iterative method used in solving Eq. [14] is explained in the following paper. Equation [14] involves the difficult function F_s, which is random in both amplitude and period, as is shown in Figures 1(a) and (b). Certain boundary conditions must be imposed at the ends of a dislocation line of total length L. The results depend upon the z dimension of the sample, but approach their asymptotic value to less than 10 pct at $z \sim 250\mathbf{b}$ and to less than 1 pct at $z \sim 500\mathbf{b}$. The length z is the minimum length of the dislocation line, *i.e.*, if it were perfectly straight. However, the dislocation does not remain straight, so the length of the dislocation is greater than the z dimension.

V. NUMERICAL RESULTS

Before beginning a discussion of the numerical results associated with the Mott limit, let us consider the



(*a*)



(*b*)

Fig. 1—(*a*) A force map for a portion of the slip plane for a dilute fcc solute solution. The vertical axis is the interaction force between the solute atoms and the dislocation line which lies along the z axis and is moving in the positive x direction. A positive force opposes the motion of the dislocation, and the negative force (the valleys) aids the motion of the dislocation in the positive x direction. (*b*) A contour force map of the same solid solution and the portion of the slip plane as shown in (a). Again the dislocation lies along the z axis and is moving in the positive x direction.

numerical results obtained for the Friedel limit or low concentration, since there is general agreement concerning the concentration dependence in the Friedel limit. Also, by considering the Friedel limit, it is possible to compare the configuration of the dislocation line as obtained by present numerical technique with that predicted by the solution of Eq. [14] using the "shooting technique."[19] (The latter technique is a numerical approach to solving differential equations with given boundary values. The solution is started at one boundary and with assumed value(s) for the lower order derivatives, the latter one used to "shoot" or bootstrap the solution numerically to the other boundary. The values of the initial derivative(s) (or "shot direction") are adjusted until the solution at the second boundary matches the required value.) It was found that the dislocation configuration was identical. In this simulation, a large misfit strain (of 0.15) and very low concentrations were used to obtain the concentration dependence of the yield stress.

As mentioned in Section II, ensuring that the concentration range is within the Friedel limit requires very small concentrations. The lower limit of the concentration that can be used in a computer simulation is determined by a limitation on the memory of our computer. The maximum size sample that can be accommodated is 5×10^6 atom sites. For a $c = 10^{-4}$, this results in 500 solute atoms. It should be pointed out that even this number of solute atoms (obstacles) is below that which is required (1000 obstacles) to ensure reasonable data.[27] Figure 2 is a plot of yield stress *vs* $c^{1/2}$ in the concentration range from 10^{-4} to 10^{-2}. For given random array, and the other parameters held constant, the variation in τ at a given concentration is very small, *i.e.*, within the data point, but if different random arrays are employed in the lowest concentration range, τ varies ±5 pct. If we consider the solid line which is a least squares fit of the data (without the requirement that at $c = 0$, $\tau = 0$), the intercept at $c = 0$ results in a positive τ. Even at the lowest concentrations ($c \sim 10^{-4}$), the data lie close to the solid line/straight line fit. Note that the yield stress must vanish at $c = 0$. Hence, the Friedel limit $\tau \sim c$ relation must be something like the dashed line in Figure 2, which distinctly deviates from the higher concentration (solid line) behavior. From this, we would conclude that the upper limit concentration of the Friedel statistics is less than 10^{-4} for the conditions of this simulation.

The above data indicate that the strengthening in the

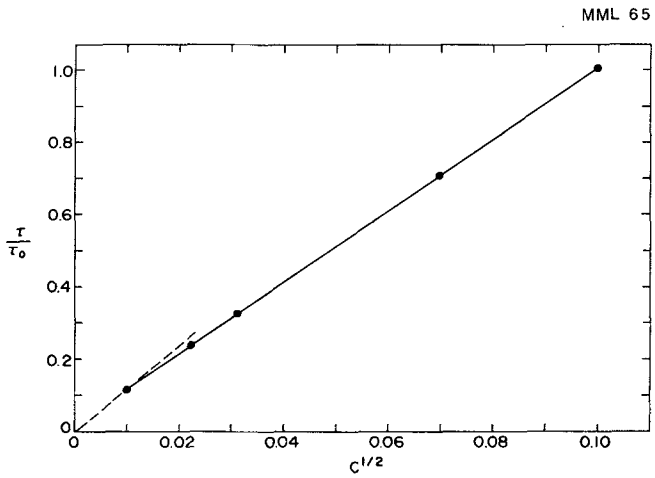


Fig. 2—A plot of the ratio of stress *vs* the yield stress at the maximum concentration as a function of concentration. The concentration range varies from $c = 10^{-4}$ to $c = 10^{-2}$. This low concentration range was chosen to approach the Friedel limit.

Friedel limit is greater than in the Mott limit. This can be understood as follows. In the Mott limit, there is considerable overlap of obstacles (cancellation of the stress fields of the solute atoms). This cancellation does not occur in the Friedel limit for incremental changes in the concentration. Hence, each new solute atom is more "efficient" in its stress field (the slope of the τ-c curve). The question arises as to whether this change in slope in the τ-c plot is detectable. We have not been able to find any experimental investigations of the yield stress at 4.2 K at concentrations below $c = 10^{-2}$, and in general, the scatter in the experimental results at low concentrations would not allow a determination as to whether the plot of τ *vs* $c^{1/2}$ should give a zero intercept at $c = 0$ or a positive value. If we consider that computer simulation data over a wider range (Figures 5 and 6), then again the change in slope at very low concentration is not detectable.

In the Mott limit, the obstacle strength (*i.e.*, misfit strain) is sufficiently weak and the concentration sufficiently high that the dislocation assumes an almost straight geometry. Various authors have disagreed over what parameter range corresponds to the Mott limit. We will adopt an empirical approach and allow the equilibrium dislocation geometry to determine when our model is in the Mott limit. Figures 3 and 4 display a typical dislocation equilibrium configuration at a concentration of 0.05 and a misfit strain of -0.01 and -0.06, respectively. At a misfit strain of -0.06, the maximum amplitude of the excursions of the dislocation in the slip direction (Δx) is less than 2**b** over a dislocation length of 100**b**. At a misfit strain of -0.01, this becomes less than 1**b**, suggesting that this is well within the Mott limit. There is an

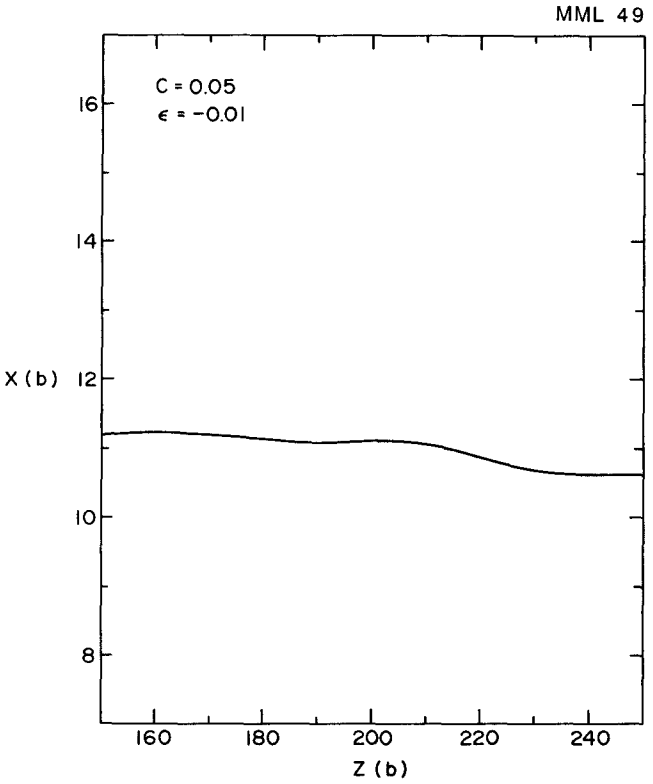


Fig. 3—A portion of the dislocation line at static equilibrium as it traverses the slip plane.

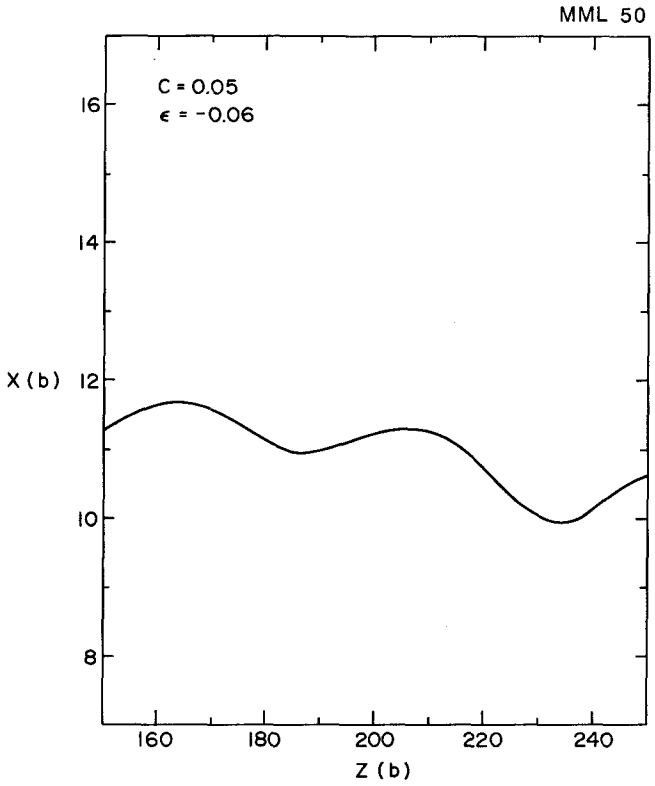


Fig. 4—A portion of a dislocation line at static equilibrium as it traverses the slip plane. This is to be compared with Fig. 3 which has a solute of a higher misfit strain.

increase in Δx_{max} (*i.e.*, maximum amplitude) with an increasing concentration. For example, at ε of 0.06, Δx_{max} increases from 0.5 to 2.6**b** as the concentration increases from 0.001 to 0.1.

In Figures 5 through 8, we present plots of yield stresses as a function of $c^{2/3}$ or as a function of $c^{1/2}$ at two different misfit strains obtained from our model. The solid circles in the figures correspond to a dislocation line length

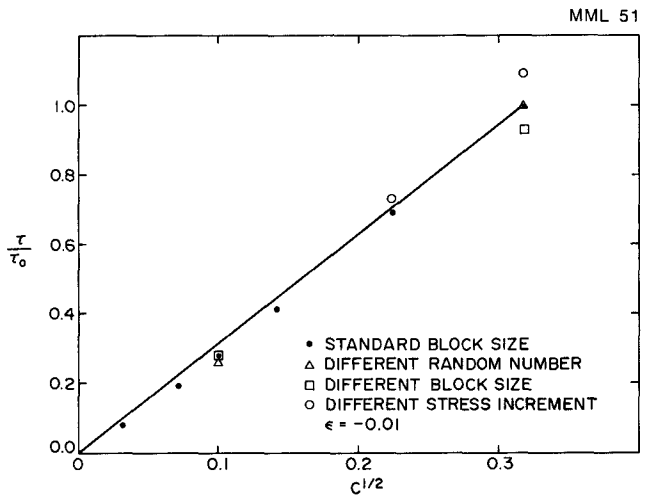


Fig. 5—A plot of the ratio of the yield stress *vs* the yield stress at the maximum concentration of 10 pct as a function of concentration. The data were obtained for different lattice sizes, *i.e.*, a different number of atoms in the lattice, different random arrays of solute atoms, and different increments of stress for the forward motion of the dislocation.

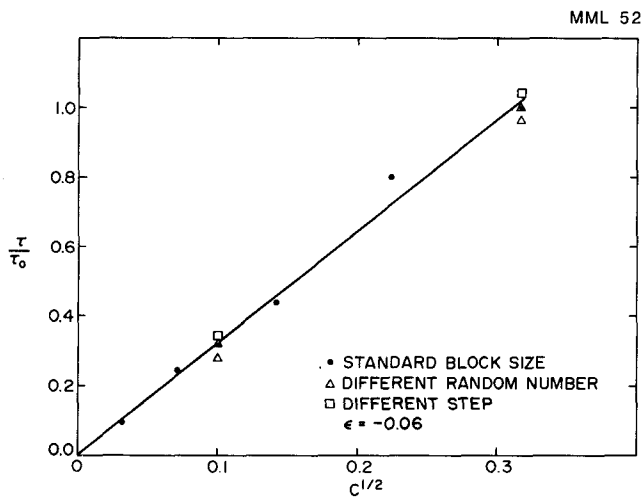


Fig. 6—A plot of the ratio of the yield stress *vs* the yield stress at the maximum concentration of 10 pct as a function of concentration. The data were obtained for different lattice sizes, *i.e.*, a different number of atoms in the lattice, different random arrays of solute atoms, and different increments of stress for the forward motion of the dislocation.

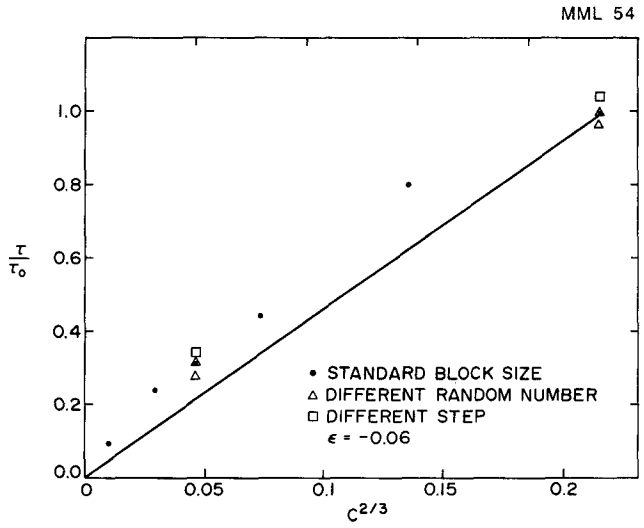


Fig. 8—A plot of the ratio of the yield stress *vs* the yield stress at the maximum concentration of 10 pct as a function of concentration. The data were obtained for different lattice sizes, *i.e.*, a different number of atoms in the lattice, different random arrays of solute atoms, and different increments of stress for the forward motion of the dislocation.

of about 500**b**. The data points (△) are also provided for a dislocation line length of about 500**b** but were obtained with a different random configuration of solute atoms. An increase in dislocation line length to about 1000**b** (□) resulted in no significant change in yield stress. A stress iteration step size that is a factor of 10 larger than that used in the generating of the other data points (○) did result in a higher stress value. As explained in the succeeding paper, the use of a coarser stress step size in the iterative solution of the equilibrium Eq. [14] leads to a less accurate solution. Inclusion of these additional data points provides some measure of the variance in our numerical results. In particular, the negligible change in the yield stress for our stress iteration step size (the solid circle *vs* open circle points) and a dislocation line length of about 500**b** *vs* about 1000**b** (the solid circle *vs* (□) points) suggest the numerical accuracy is quite satisfactory.

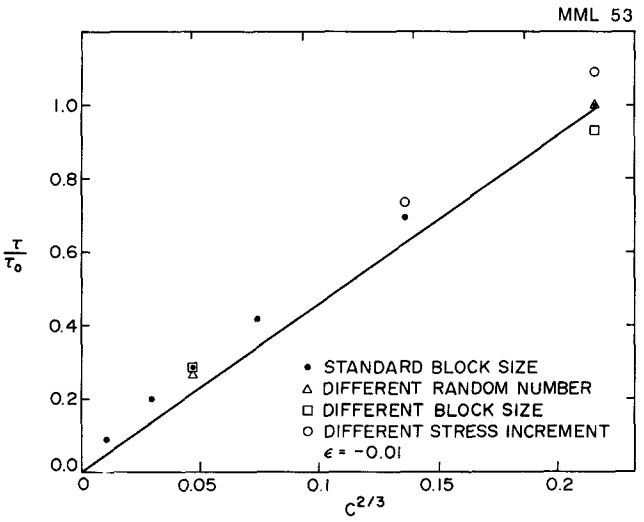


Fig. 7—A plot of the ratio of the yield stress *vs* the yield stress at the maximum concentration of 10 pct as a function of concentration. The data were obtained for different lattice sizes, *i.e.*, a different number of atoms in the lattice, different random arrays of solute atoms, and different increments of stress for the forward motion of the dislocation.

Included in Figures 5 through 8 are straight lines connecting the origin (zero concentration, zero yield stress) with the closed circle data point at a concentration of 0.10. All of the data plots in these figures are within the Mott limit, if the Mott is defined as the condition such that amplitude of the dislocation fluctuation is $<2\mathbf{b}$. It is clear from Figures 5 and 6 that the simple straight line fit to a $c^{1/2}$ power law works remarkably well over the ENTIRE concentration range—with one constant of proportionality. In contrast, Figures 7 and 8 indicate that a $c^{2/3}$ power law provides a substantially worse fit over the entire concentration range. A least squares fit of the data in Figures 7 and 8 results in a reasonable straight line fit, but at zero concentration, a positive value of stress is predicted. A nonzero value of stress is not possible at zero concentration.

Of course, the analytical models predict a $c^{2/3}$ behavior only in the Mott limit. Kocks *et al.*[20] suggest the Mott limit begins at a concentration of about 0.002 at a misfit strain of 0.01 and at a concentration of about 0.005 at a misfit strain of 0.06. Labusch places these limits at even lower concentrations: about 0.0001 and 0.001, respectively. If we accept the Labusch estimates, all of our data points are in the Mott limit.

It may be argued that the computer simulation data do result in a reasonable fit of $c^{2/3}$ dependence (Figure 9), and at low concentrations, the Friedel statistics apply, as indicated by the dashed line in Figure 9. However, here the change in slope going from the Friedel limit (dashed line) to the Mott limit ($c^{2/3}$ solid line) in Figure 9 is quite drastic. While he argued earlier that the incremental strengthening in the Friedel limit is greater than the incremental strengthening in the Mott limit, the

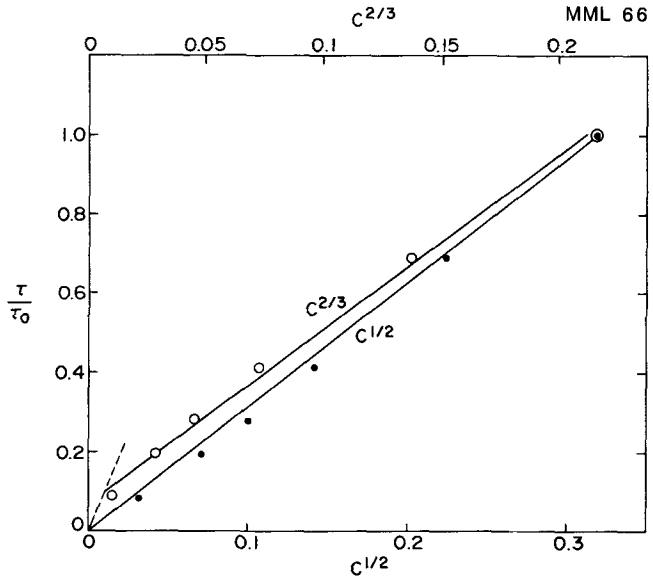


Fig. 9—A combined plot of the yield stress *vs* the combined plot of the ratio of the yield stress *vs* the yield stress at the maximum concentration as a function of concentration. Two different concentration dependencies are shown, and these are $c^{2/3}$ and $c^{1/2}$.

change in the slopes required of the two curves is, in our opinion, unreasonably large.

VI. CONCLUSION

A detailed consideration of the Friedel and Mott limits was undertaken to determine whether the previously assumed concentration dependencies for these limits were valid.

As is to be expected, the data obtained both analytically and numerically in the Friedel limit agree with the previously assumed concentration dependence of $c^{1/2}$. However, in the case of the Mott limit, numerous assumptions had to be made by previous investigators in order to obtain an analytical solution. One of these assumptions was that the yield stress should be equated to the *average* of interaction force between the solute atom and the dislocation. The average force over a very long dislocation line is equal to zero. If the yield stress is equated to the root mean square of the interaction force, then a concentration dependence of $c^{1/2}$ is obtained for the Mott limit. Further extensive numerical analysis results in a confirmation of a $c^{1/2}$ concentration dependence for the Mott limit.

ACKNOWLEDGMENTS

One of the authors (R.J.A.) would like to acknowledge the extended support given by the Computer Science Center of the University of Maryland. This research was supported in part by the National Science Foundation under Grant No. DMR-82-04059.

REFERENCES

1. H. Suzuki: *Dislocations and Mechanical Properties of Crystals*, John Wiley & Sons, New York, NY, 1957, p. 361; *Strength of Metals and Alloys*, Pergamon Press, New York, NY, 1985, vol. 3, p. 1727.
2. M.Z. Butt and P. Feltham: *Reviews on the Deformation Behavior of Metals*, 1978, vol. III, p. 99.
3. N.F. Mott and F.R.N. Nabarro: Report of a Conference on the Strength of Solids, F, University of Bristol, England, Physical Society, London, 1948.
4. R.L. Fleischer: *Acta Metall.*, 1961, vol. 9, p. 996; 1963, vol. 11, p. 203.
5. R.L. Fleischer: *Acta Metall.*, 1962, vol. 10, p. 855.
6. R.L. Fleischer: *The Strengthening of Metals*, Reinhold Publ. Co., New York, NY, 1964, p. 93.
7. J. Friedel: *Dislocations*, Addison-Wesley Publ. Co., Reading, MA, 1964.
8. R. Labusch: *Phys. Stat. Sol.*, 1970, vol. 41, p. 659; *Acta Metall.*, 1972, vol. 20, p. 917.
9. R. Labusch: *Rate Processes in Plastic Deformation of Materials*, Proc. from the J.E. Dorn Symp., Plenum Press, New York, NY, 1975, p. 26.
10. T. Suzuki: *Dislocation Dynamics*, McGraw-Hill, New York, NY, 1968, p. 551.
11. O. Boser: *Metall. Trans.*, 1972, vol. 3, pp. 843-49.
12. O. Boser: *J. Appl. Phys.*, 1973, vol. 44, pp. 1033, 1038.
13. B.R. Riddhagni and R.M. Asimow: *J. Appl. Phys.*, 1968, vol. 30, p. 4144; 1968, vol. 39, p. 6159.
14. W.R. Tyson: *Physics of Solid Solution Strengthening*, Plenum Press, New York, NY, 1973, p. 47.
15. A.H. Cottrell, S.C. Hunter, and F.R.N. Nabarro: *Phil. Mag.*, 1953, vol. 44, p. 1064.
16. F.R.N. Nabarro: *J. Less-Common Metals*, 1972, vol. 29, p. 257.
17. F.R.N. Nabarro: *Phil. Mag.*, 1977, vol. 35, p. 613.
18. F.R.N. Nabarro: *Dislocation and Properties of Real Materials*, The Institute of Metals, London, 1985, p. 152.
19. R.J. Arsenault, R. Hsu, and D. Esterling: *Scripta Metall.*, 1981, vol. 15, p. 567.
20. U.F. Kocks, A.S. Argon, and M.F. Ashby: *Thermodynamics and Kinetics of Slip in Prog. in Mat. Sci.*, Pergamon Press, Oxford, 1975, vol. 19.
21. U.F. Kocks: *Metall. Trans. A*, 1985, vol. 16A, pp. 2109-29.
22. A.J.E. Foreman and M.J. Makin: *Phil. Mag.*, 1966, vol. 14, p. 911.
23. A.J.E. Foreman and M.J. Makin: *Canadian J. Phys.*, 1967, vol. 45, p. 511.
24. *Proc. 1976 Int. Conf. on Computer Simulation for Materials Applications*, R.J. Arsenault, J.R. Beeler, Jr., and J.A. Simmons, eds., NBS, Gaithersburg, MD, April 1976: R. Labusch and R.B. Schwartz, vol. 2, p. 650; S.I. Zaitsev and E.M. Nadgornyi, vol. 2, p. 707; R.O. Scattergood and E.S.P. Das, vol. 2, p. 740; K. Hanson, S. Altintas, and J.W. Morris, Jr., vol. 2, p. 917.
25. R.J. Arsenault and T.W. Cadman: *Phil. Mag.*, 1970, vol. 24, p. 259; *Scripta Metall.*, 1973, vol. 6, p. 593; *Scripta Metall.*, 1973, vol. 7, p. 631; *Phys. Stat. Sol.*, 1974, vol. 24, p. 299; *Rate Processes in Plastic Deformation*, ASM, 1975, vol. 4, p. 102; *Scripta Metall.*, 1978, vol. 12, p. 633; *Metall. Trans. A*, 1980, vol. 11A, pp. 127-34; *Scripta Metall.*, 1981, vol. 15, p. 995; *Scripta Metall.*, 1984, vol. 18, p. 495.
26. K. Ono: Proc. of the 3rd Int. Conf. on the Strength of Metals and Alloys, Cambridge, England, 1973.
27. C.T.K. Kuo and R.J. Arsenault: *Mater. Sci. Eng.*, 1976, vol. 27, p. 11; 1977, vol. 30, p. 65.
28. R.B. Schwartz and R. Labusch: *J. Appl. Phys.*, 1978, vol. 49, p. 5174.
29. D.M. Esterling and R.J. Arsenault: *Metall. Trans. A*, 1982, vol. 13A, pp. 1429-34.
30. W.E. Nixon and J.W. Mitchell: *Proc. Royal Soc. London*, 1981, vol. 376A, p. 343.