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Mobility of arrays of dissociated and superlattice dislocations in an internally stressed solid

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A study is made of the mobility of planar arrays of dislocations of Burgers vector b that are either separated into their component partials or are of the superlattice type and are contained in an internally stressed solid, the stress being generated by a preexisting coplanar obstacle dislocation of Burgers vector mb. The aim here is to estimate the effect of the internal stress and the fault energy on the separation between the components of the first discrete dislocation since the latter plays an important part in a wide range of physical phenomena. All the mobile complete dislocations except the leader are either smeared into a continuous distribution or are replaced by a superdislocation of appropriate Burgers vector. These two approaches, which lead to lower and upper bounds for the separation distance, are shown to give fairly close results for small m.

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I. INTRODUCTION

In practice, there are many situations in which planar arrays of dislocations propagate through an internally stressed solid, the internal stress being generated by preexisting locked dislocations. In such situations the internal stress may vary significantly over a distance comparable with the spacing between leading mobile dislocations. Furthermore, recent interest in the yield and fracture characteristics of alloys has led to the formulation of theoretical models[1–3] in which complete dislocations in the array are either separated into energetically favorable partials or are of the superlattice type, a complete mobile dislocation being associated in each case with a faulted region characterized by an energy parameter γ, the aim being to study the part played by the latter in these physical phenomena.

As with the classical dislocation pileups, several approaches are theoretically feasible for analyzing such models. Thus, Li[4] used the discrete dislocation pileup model[5] in studying the effect of alloy additions on the relation between the yield stress and the grain size of a polycrystalline material. This approach has the distinct advantage of preserving the physical reality of the given situation but requires an appreciable computational effort if the number of free dislocations is very large. At the other extreme is the approach whereby all the free dislocations are smeared into a continuous distribution, an appropriate distribution function describing the resulting dislocation density.[6,7] This approach, though mathematically simple, deviates considerably from the physical situation.[8]

With the distinct advantages of these two extreme approaches in mind, Smith[9] proposed an elegant mixed discrete-continuous model in which a majority of the free dislocations in the array are smeared into a continuous distribution, while those that are intimately concerned with the particular physical phenomenon under consideration are allowed to remain discrete, thereby retaining the physical reality of the discrete model and the mathematical simplicity of the continuous distribution approach. The mixed model has found many useful applications.[10]

In the light of the above considerations it was thought clearly desirable to extend this approach to the case of an array of superlattice and dissociated dislocations propagating through an internally stressed solid. Moreover, an alternative approach has been employed whereby all but the leading mobile complete dislocation are replaced by a superdislocation of appropriate Burgers vector. It is shown that the results of the two methods are in good agreement for small m, mb being the Burgers vector of the barrier dislocation.

II. THEORETICAL ANALYSIS

A. Mixed model

The theoretical model illustrated in Fig. 1, consists of n positive complete edge dislocations (screws are briefly considered later) lying in the plane $y=0$. Each dislocation has a Burgers vector b, and the associated extra half-plane of atoms is in the positive y direction. Each edge dislocation is dissociated into two energetically favorable partials that have Burgers vectors inclined at an angle θ to the vector of the complete dislocation and that bound a ribbon of stacking fault whose energy is γ. The array of dissociated dislocations is moving towards a locked coplanar complete edge dislocation of Burgers vector mb under the action of an externally applied shear stress $p_{xy}=\sigma$. In accordance with the

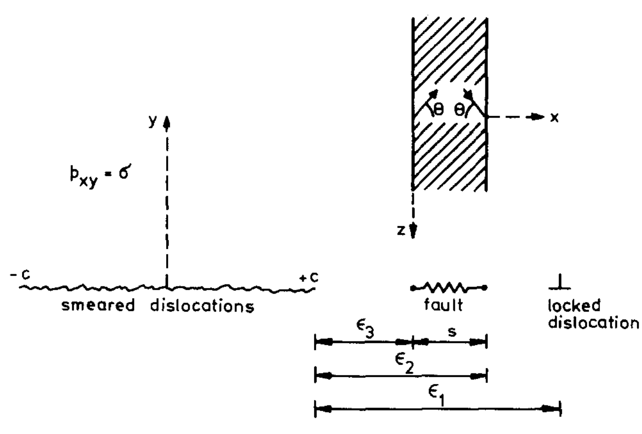

FIG. 1. Mixed continuous–discrete extended edge dislocation model together with a locked edge dislocation.

mixed model, the first complete mobile dislocation with its leading and trailing partials situated at $x=c+\epsilon_2$, $y=0$, and $x=c+\epsilon_3$, $y=0$, respectively, is allowed to remain discrete, while the remaining $(n-1)$ complete edge dislocations are smeared into a continuous distribution within the interval $|x| \leq c$, $y=0$, it being implied that the latter possess no faults. The barrier dislocation of the same orientation is situated at $x=c+\epsilon_1$, $y=0$. Then the appropriate function $f(x)$ describing the distribution density of the smeared dislocations satisfies the singular integral equation

$$\int_{-c}^{c} \frac{f(\lambda)\,d\lambda}{x-\lambda} + \frac{\sigma}{A} + \frac{1}{2[x-(c+\epsilon_2)]} + \frac{1}{2[x-(c+\epsilon_3)]} + \frac{m}{x-(c+\epsilon_1)} = 0 \tag{1}$$

for $|x| \leq c$, the Cauchy principal value of the singular integral being implied to avoid divergence at $x=\lambda$; A is equal to $\mu b/2\pi(1-\nu)$, where μ is the shear modulus and ν Poisson's ratio. $f(x)$ is bounded at $x=\pm c$ provided that[11]

$$\int_{-c}^{c} \left(\frac{\sigma}{A} + \frac{1}{2[x-(c+\epsilon_2)]} + \frac{1}{2[x-(c+\epsilon_3)]} + \frac{m}{x-(c+\epsilon_1)}\right) \frac{dx}{(c^2-x^2)^{1/2}} = 0, \tag{2}$$

the solution of (1) being

$$f(x) = \frac{(c^2-x^2)^{1/2}}{2\pi[(c+\epsilon_2)^2-c^2]^{1/2}[(c+\epsilon_2)-x]} + \frac{(c^2-x^2)^{1/2}}{2\pi[(c+\epsilon_3)^2-c^2]^{1/2}[(c+\epsilon_3)-x]} + \frac{m(c^2-x^2)^{1/2}}{\pi[(c+\epsilon_1)^2-c^2]^{1/2}[(c+\epsilon_1)-x]}. \tag{3}$$

The existence condition (2) simplifies to

$$\frac{\sigma}{A} = \frac{1}{2[\epsilon_2(2c+\epsilon_2)]} + \frac{1}{2[\epsilon_3(2c+\epsilon_3)]^{1/2}} + \frac{m}{[\epsilon_1(2c+\epsilon_1)]^{1/2}}, \tag{4}$$

while the total number of complete mobile dislocations is obtained from (3) as

$$n = 1 + \int_{-c}^{c} f(x)\,dx. \tag{5}$$

Since both the trailing and the leading partials of the discrete extended edge dislocation are also in equilibrium,

$$\int_{-c}^{c} \frac{f(x)\,dx}{(c+\epsilon_3)-x} + \frac{\sigma}{A} + \frac{2\gamma}{bA} - \frac{1}{2(\epsilon_2-\epsilon_3)}[1-(1-\nu)\tan^2\theta] - \frac{m}{\epsilon_1-\epsilon_3} = 0, \tag{6a}$$

$$\int_{-c}^{c} \frac{f(x)\,dx}{(c+\epsilon_2)-x} + \frac{\sigma}{A} - \frac{2\gamma}{bA} + \frac{1}{2(\epsilon_2-\epsilon_3)}[1-(1-\nu)\tan^2\theta] - \frac{m}{(\epsilon_1-\epsilon_2)} = 0. \tag{6b}$$

If the number of mobile dislocations n is large, ϵ_2 and ϵ_3 will both be small compared with c. Furthermore, if $n \gg m$, ϵ_1 is also small in comparison with c and expressions (4)–(6) are appreciably simplified. Now, if the spacing between the partials of the discrete extended dislocation is designated by $s=\epsilon_2-\epsilon_3=k_1\epsilon_3$ and the distance between the locked dislocation and the trailing partial by $s_1=\epsilon_1-\epsilon_3=k_2\epsilon_3$, relations (4) and (5), after simplification, give

$$s = (k_1 A/8n\sigma)[1+(1+k_1)^{-1/2}+2m(1+k_2)^{-1/2}]^2, \tag{7}$$

while expressions (6) establish a relationship between k_1 and k_2:

$$\frac{(1+k_2)^{1/2}}{2}\left((1+k_1)^{1/2}+1+\frac{k_1}{2}\right) = \frac{m(1+k_1)}{k_2} + \frac{m(1+k_1)^{3/2}}{k_2-k_1}. \tag{8}$$

Expression (7) gives the separation s between the partials forming the discrete complete dislocation under the action of an applied stress σ required to bring the trailing partial to within a distance s_1 of the barrier dislocation, s and s_1 being related through (8). On the other hand, experimental data usually pertain to the equilibrium separation s_0 when the dissociated discrete edge dislocation is alone in an otherwise unstressed solid,

$$2\gamma/bA = (2s_0)^{-1}[1-(1-\nu)\tan^2\theta], \tag{9}$$

whereupon expressions (6a) and (9) give

$$(1+k_1)^{-1/2} - \tfrac{1}{2}k_1 + (2mk_1/k_2)(1+k_2)^{-1/2} = \lambda_1, \tag{10}$$

where

$$\lambda_1 = s/s_0 + (1-\nu)(1-s/s_0)\tan^2\theta. \tag{11}$$

Furthermore, (7) and (9), together with (10), give the stress σ required to bring the trailing partial to within a distance $s_1=k_2\epsilon_3$ of the obstacle:

$$\frac{n\sigma b}{\gamma} = \frac{[1+(1+k_1)^{-1/2}+2m(1+k_2)^{-1/2}]^2 k_1}{2[(1+k_1)^{-1/2}-\frac{1}{2}k_1+(2mk_1/k_2)(1+k_2)^{-1/2}-(1-\nu)\tan^2\theta]}. \tag{12}$$

In practice, a value of λ_1 (i.e., s/s_0 for given ν and θ) is specified and the system of nonlinear equations (8) and (10) is solved numerically subject to the condition $k_2 > k_1$.[12] The stress σ required to achieve this state is then calculated from (12). The preceding relations are equally applicable in the case where both extended mobile dislocations and the barrier are of the screw orientation and are subjected to an external shear stress $p_{yz}=\sigma$. It is only necessary to set A equal to $\mu b/2\pi$ instead of $\mu b/2\pi(1-\nu)$ and replace $(1-\nu)$ by $(1-\nu)^{-1}$ in all the relations.

From physical arguments[13] it is clear that expression (12) gives the lower bound for the stress σ. It is also known[1] that the upper bound for the stress σ (or s/s_0) is analogous to that obtained by the superdislocation approach. That the superdislocation model should give an upper bound seems to be in agreement with the results of Hazzledine and Hirsch,[14] who have shown that the most effective obstacle action is confined to small regions near the rear of the pileup, well removed from its "center of gravity" (at which the superdislocation is assumed to be situated).

B. Superdislocation model

As mentioned above, if all but the leading mobile

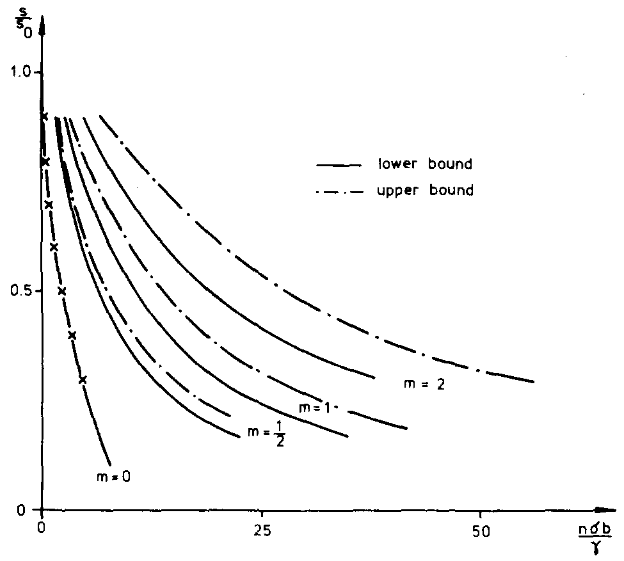

FIG. 2. Upper and lower bounds for the separation distance s between the partials of the leading extended edge dislocation for various values of m. s_0 is the spacing between the partials in an unstressed lattice.

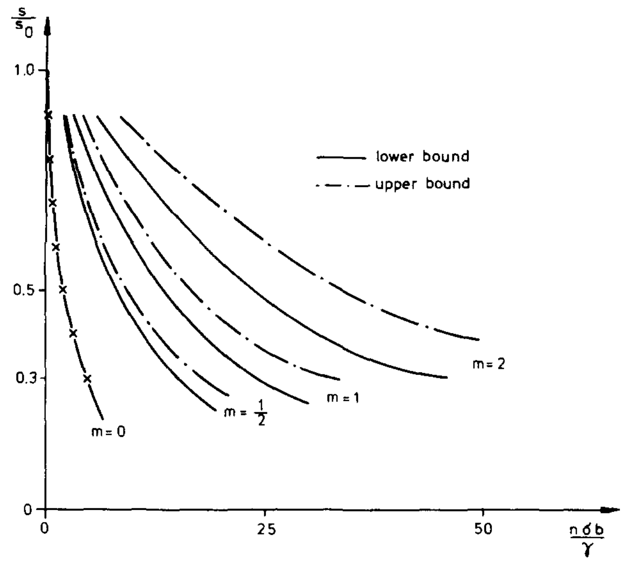

FIG. 3. Upper and lower bounds for the separation distance s between the partials of the leading extended screw dislocation for various values of m. s_0 is the spacing between the partials in an unstressed lattice.

complete edge dislocations, instead of being smeared into a continuous distribution, are replaced by a superdislocation of Burgers vector $(n-1)b$, then the situation (when $n \gg m$) is equivalent to that of a single complete dislocation being subject to a stress which maintains the superdislocation in equilibrium,

$$\sigma = (m+1)A/d, \tag{13}$$

where d is the distance between the superdislocation and the trailing partial of the discrete complete dislocation and is assumed to be much larger than ϵ_1, ϵ_2, or ϵ_3.

Furthermore, since both the trailing and the leading partials of the discrete complete edge dislocation are also in equilibrium,

$$\frac{\sigma}{A} + \frac{(n-1)}{d+\epsilon_3} + \frac{2\gamma}{bA} - \frac{1}{2(\epsilon_2-\epsilon_3)}[1-(1-\nu)\tan^2\theta] - \frac{m}{\epsilon_1-\epsilon_3} = 0, \tag{14}$$

$$\frac{\sigma}{A} + \frac{(n-1)}{d+\epsilon_2+\epsilon_3} - \frac{2\gamma}{bA} + \frac{1}{2(\epsilon_2-\epsilon_3)}[1-(1-\nu)\tan^2\theta] - \frac{m}{\epsilon_1-\epsilon_2} = 0.$$

The comments made above regarding the screw dislocations also hold good in the present case.

By using (14) and (9) it is easy to show that $k = k_1/k_2$ is given by

$$k = -\frac{\lambda_2}{2m} + \left(\frac{\lambda_2^2}{4m^2} + \frac{\lambda_2}{m}\right)^{1/2}, \tag{15}$$

where

$$\lambda_2 = (1 - s/s_0)[1-(1-\nu)\tan^2\theta]. \tag{16}$$

Also using one of the two expressions (14) and (9) it follows that

$$\frac{n\sigma b}{(m+1)\gamma} = \frac{4(s_0/s)\{\frac{1}{2}[1-(1-\nu)\tan^2\theta] + mk\}}{1-(1-\nu)\tan^2\theta} - 2. \tag{17}$$

As mentioned above, (17) gives the upper bound for the stress σ.

At this stage it is instructive to specialize the results of the two approaches to particular cases of pileups of dissociated dislocations in fcc structure.

III. SPECIAL CASE OF THE fcc STRUCTURE

A. Edge- and screw-type extended dislocations

When both the barrier and the mobile extended dislocations have edge (screw) orientation, then in fcc materials total dislocations of Burgers vector $(a/2)$ $[1\bar{1}0]$ can dissociate into a pair of Shockley partial dislocations with Burgers vector $(a/6)$ $[1\bar{2}1]$ and $(a/6)$ $[2\bar{1}\bar{1}]$ separated by a region of stacking fault on the (111) plane, the angle θ being equal to 30°. The equilibrium spacing s_0 between the partials in the unstressed lattice for $\nu = \frac{1}{3}$ is given by (9):

$$\begin{aligned} 2\gamma/bA &\simeq 7/18 s_0 \quad \text{(edges)}, \\ &\simeq 1/4 s_0 \quad \text{(screws)}, \end{aligned} \tag{18}$$

γ being the stacking fault energy.

Furthermore, the parameters λ_1 and λ_2 are given by

$$\begin{aligned} \lambda_1 &= \tfrac{2}{9}(1 + \tfrac{7}{2}s/s_0) \quad \text{(edges)} \\ &= \tfrac{1}{2}(1 + s/s_0) \quad \text{(screws)}, \\ \lambda_2 &= \tfrac{7}{9}(1 - s/s_0) \quad \text{(edges)} \\ &= \tfrac{1}{2}(1 - s/s_0) \quad \text{(screws)}. \end{aligned} \tag{19}$$

The lower and upper bounds for σ (and by implication for s/s_0) for various values of m given by Eqs. (12) and (17) for dislocations of edge and screw orientations are shown in Figs. 2 and 3, respectively. Results for $m=0$ were obtained earlier.[1] As the bounds are close to each other for small values of m, the separation distance s may be accurately estimated for a given applied stress σ.

B. Pileup of superlattice dislocations

If each superlattice dislocation consists of a pair of

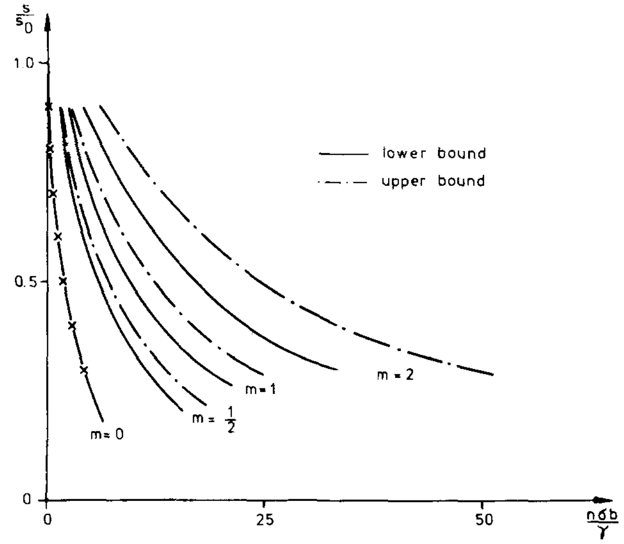

FIG. 4. Upper and lower bounds for the separation distance s between the components of the leading superlattice edge dislocation for various values of m. s_0 is the spacing between the components in an unstressed lattice.

perfect edge dislocations, θ is equal to zero and the antiphase boundary connecting the two dislocations corresponds to the stacking fault with energy γ given by [Eq. (9)]

$$2\gamma/bA = 1/2s_0. \tag{20}$$

Equations (7), (20), and (12) simplify to

$$\frac{s}{s_0} = 1 - \left(1 + \frac{k_1}{2} - (1+k_1)^{-1/2} - 2m\frac{k_1}{k_2}(1+k_2)^{-1/2}\right), \tag{21}$$

$$\frac{n\sigma b}{\gamma} = \frac{[1 + (1+k_1)^{-1/2} + 2m(1+k_2)^{-1/2}]^2 k_1}{2[(1+k_1)^{-1/2} - \frac{1}{2}k_1 + 2m(k_1/k_2)(1+k_2)^{-1/2}]}, \tag{22}$$

k_1 and k_2 being determined as before by (8) and (10) with $\lambda_1 = s/s_0$.

The upper bound for the stress σ is given by the superdislocation approach [Eq. (17)]:

$$n\sigma b/(m+1)\gamma = 4(s_0/s)(\tfrac{1}{2} + mk) - 2, \tag{23}$$

k being determined as before by (15) with $\lambda_2 = (1 - s/s_0)$. [Note that if the superlattice dislocation with Burgers vector b is composed of a pair of perfect screw dislocations, each with a Burgers vector $\frac{1}{2}b$, the preceding relations hold good with A taking the value $\mu b/2\pi$ instead of $\mu b/2\pi(1-\nu)$.]

The upper and lower bounds for σ (and by implication for s/s_0) for various values of m are shown in Fig. 4. As before, the bounds are fairly close to each other for small values of m allowing the separation s between the components forming the leading superlattice dislocation to be determined rather accurately for a given applied stress σ in terms of the equilibrium spacing s_0 between the components in an unstressed lattice. Here it may be instructive to consider the special case when there is no long-range order, i.e., $\gamma = 0$. In this case, k_1 and k_2 may be calculated from (8) and (10) with $\lambda_1 = 0$. The distance $s_2 = \epsilon_1 - \epsilon_2 = (k_2 - k_1)\epsilon_3$ to within which the leading component of the discrete superlattice dislocation approaches the locked dislocation under a given applied stress σ may then be readily evaluated from an expression similar to (7):

$$s_2 = [(k_2 - k_1)A/8n\sigma][1 + (1+k_1)^{-1/2} + 2m(1+k_2)^{-1/2}]^2. \tag{24}$$

The situation here is identical to the propagation of edge dislocations, each of Burgers vector b, in an internally stressed solid. This model has been analyzed exactly (all the dislocations allowed to remain discrete) by Chou[15] for $n = 8$, the distance to which the leader in the mobile group approaches the fixed dislocation being given by $Aq_{1,n}/2\sigma$, where $q_{1,n}$ is the first zero of the generalized Laguerre polynomial L_n^{2m-1}. With $n = 8$, $q_{1,n}$ has the values 0.41, 1.03, and 1.79 for $m = 1, 2, 3$, whereas the present technique gives s_2 (in units of $A/2\sigma$) as 0.35, 0.92, and 1.60, respectively. The agreement is fairly good even for $m = 3$.

IV. DISCUSSION

The primary objective of this paper has been to extend the use of the mixed discrete-continuous (compromise) dislocation model to situations where the complete dislocations in a planar array are either split into components bounding a certain ribbon of fault characterized by an energy parameter or are of the superlattice type. The first complete dislocation was allowed to remain discrete and to possess an associated fault, while the remaining mobile dislocations in the array were smeared into a continuous distribution as if their fault energy were infinite, the aim being to study the influence of an externally applied shear stress and an internal stress (generated by a preexisting locked dislocation) on the separation between the partials forming the first complete dislocation. Additionally, a very simple approach has also been employed in which all but the leading complete dislocation in the mobile array, instead of being smeared into a continuous distribution, are replaced by a superdislocation with an appropriate Burgers vector. The results of these two approaches were specialized to situations arising in the fcc structure and to the pileup of superlattice dislocations. These two approaches give the lower and upper bounds for the separation distance, it being demonstrated that the bounds are close to each other for small values of m, where m is the ratio of the Burgers vector of the locked dislocation to that of the complete mobile dislocation, thus allowing an accurate estimate to be made of the separation distance between the partials of the discrete mobile dislocation for a given applied shear stress.

The specific form of the barrier considered here, namely a preexisting dislocation coplanar with and parallel to the mobile dislocations, clearly plays a prominent role in physical phenomena like cross-slip. Thus, cross-slip is more difficult in this case than if the barrier were the leading partial of the first complete dislocation because the repulsive force due to the barrier acts not only on the leading but also on the trailing partial. The model is equally suited for investigating crack nucleation and cross-slip phenomena in the vicinity of other barriers like point defects, grain boundaries, etc. Moreover, the strength of the barrier could be varied so as to simulate residual stress and prestraining effects. In this connection it is worth noting that stress-induced changes in the separation of the partial dislocations contribute to the energy storing capacity of Cu-Al alloys, and the greater the Al content the greater this capacity.[16] As the stacking fault energy of Cu-Al alloys decreases with increasing content of Al, the results of the present investigation could be adopted to study the change in the energy-storing capacity of such alloys since this capacity evidently plays an important part in their observed yield behavior.

Here, it may be mentioned that there are situations where the dislocations at the tail of a dislocations array could have a direct role to play (for example, in work hardening) through the back stresses created during pileup. This would require an examination of the discrete complete dislocations at the tail of a pileup. This has been omitted in the present investigation mainly because experimental evidence[16] pertaining to Cu-Al with the fcc structure suggests otherwise, namely that the back stresses created during pileup are not large enough to create a backward motion of dislocations during unloading.

In addition, the lower bound procedure used here can easily be extended to cover the case of unlike dislocations[17] whose mutual annihilation is a likely cause of the low work-hardening rate in stage III. However, the superdislocation approach can obviously not be applied.

Finally, it may be mentioned that the results obtained by the lower bound procedure find a direct application[18] in estimating the stress needed by the mobile array of dissociated (superlattice) dislocations to bypass a noncoplanar obstacle. Such estimates are useful in discussing the large strain flow behavior of fcc metals and alloys.[18]

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[12] An appropriately chosen initial value of k_2 that guarantees convergence permits reduction of (8) to a cubic in k_1. The root of the cubic satisfying the physical requirement $k_2 > k_1$ allows (10) to be rearranged as a fifth-order polynomial in k_2. With the new value of k_2 obtained by solving this fifth-order polynomial, a fresh iteration is started and the process continued until the difference of the successive iterates is less than a specified allowable error (0.5%). In all the cases reported in the present paper no nonuniqueness was encountered, there being only one pair of values (k_1, k_2) that satisfied the physical requirement $k_2 > k_1$.
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