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Dislocation behaviour in ordered alloys in the presence of frictional forces

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A detailed numerical analysis has been made of the passing of superlattice dislocations in the presence of frictional forces and the results compared with those for ordinary dislocations. In particular, it was shown that the behaviour of superlattice dislocations is similar to that of ordinary dislocations, only at very high frictional stresses or at very low vertical separations. It was also shown that dipole strength can be increased significantly by decreasing y, the vertical separation, until y reaches a critical value, y_c, when the cross-slip forces due to the internal stresses are sufficient to induce non-thermal cross-slip thus annihilating the passing dislocations. Edge dislocations, on the other hand, cannot annihilate themselves by climb, and hence, smaller vertical separation can be obtained increasing the dipole strength significantly. The effect of thermal and nonthermal cross-slip on the work-hardening of ordered alloys is discussed in detail. For the purpose of illustration, the calculations were made for FeCo. The results, however, are quite general and are applicable to all B2-structure alloys.

1. Introduction

Because of the presence of antiphase boundaries (APB) the deformation in ordered single crystalline alloys is mostly restricted to one or two slip systems [1-3]. Furthermore, in such alloys a recovery process like cross-slip is much more difficult since it involves the creation of high energy APB on the cross-slip plane [4, 5]. Hence, atomic ordering causes two pronounced changes in the macroscopic stress-strain behaviour; it induces a high work-hardening though the slip activity is restricted to one or two slip systems [1-3], and it also induces large overshoot in the slip system, when single crystals are oriented for single slip [6]. Hence, ordered alloys are particularly suited to investigate the mechanism of work-hardening in metals and alloys where there is only a single slip system. The high work-hardening observed in such alloys was accounted for by Vidoz and Brown [7] and Schoeck [8, 9] as due to the creation of APB tubes when glide dislocations intersect forest dislocations. However, to date, there has been no convincing evidence showing the presence of such APB tubes in these alloys. On the other hand, it has been well documented in the literature that most of the dislocations in ordered alloys are essentially locked as dipoles [1-3]. Though we do not rule out the formation of such APB tubes, nor their contribution to the work-hardening in ordered alloys, we believe, however, that most of the work-hardening results from the locking of passing dislocations as dipoles. With this in mind, a detailed analysis of the behaviour of dislocations passing one another on parallel slip planes in superlattices has been made [10, 11]. In particular, the analysis showed that dislocations do not pass one another as a full superlattice dislocation if the vertical separation is below a critical value. For such small vertical separations, the stress to break a dipole is much greater than the stress necessary to create APB and, hence, splitting of the partials comprising a superlattice dislocation occurs in preference to dipole breaking. In view of the importance of such calculations to the theory of work-hardening, they have been extended to include large arrays of dislocations. In particular, calculations have been previously carried out for large arrays of dislocations in disordered alloys [12, 13] using frictional forces [14] to stabilize

these dislocations. Based on the results of such calculations, a work-hardening model [13] was presented for disordered alloys. This model was extended to the case of ordered alloys. However, a detailed understanding of the behaviour of passing dislocations in ordered alloys in the presence of lattice frictional forces is still lacking. In the present paper an analysis of the behaviour of passing dislocations in superlattices in the presence of frictional forces is presented. We consider here only the case involving a pair of superlattice dislocations in order to bring out most of the concepts involved. The treatment of larger arrays of superlattice dislocations will be considered in a future study.

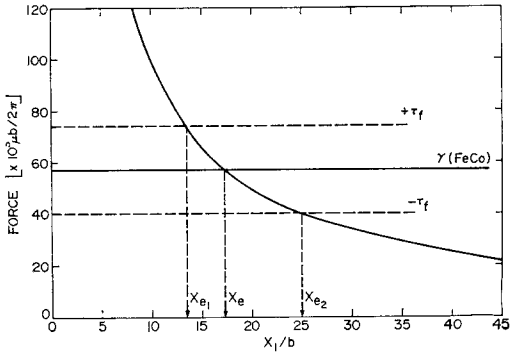


Figure 1 Equilibrium configuration of a superlattice dislocation in the presence of frictional forces.

2. Superlattice dislocations

It was pointed out earlier [15] that there are two limiting equilibrium configurations for a superlattice dislocation in the presence of frictional forces, depending upon how the APB is formed. This point is illustrated in Fig. 1, where the force between two partials is plotted as a function of their separation, x_1. Because of APB tension, the two partials spread apart to $x_1 = x_e$, where their repulsive forces are equal to γ, the APB energy. For illustration, γ of FeCo[16] is used in Fig. 1. In the presence of a frictional force corresponding to τ_f, there are two equilibrium positions; one on either side of x_e. They correspond to the positions where the total force on each dislocation is equal to the opposing frictional force, and they are termed the limiting equilibrium positions. They are so called because any position between the two limiting positions is stable since the total force on each dislocation for such a configuration is less than the friction force [14]. If the frictional stress is greater than γ, the equilibrium corresponding to the upper limit (x_{e_2}) tends to infinity, implying all values of x_1 greater than x_{e1} are stable. On the other hand, if γ tends to zero, corresponding to a disordered alloy, there is no equilibrium position between the two partials in the absence of frictional forces since there are only repulsive forces between the dislocations. In the presence of friction, however, there will be only one limiting equilibrium [15] corresponding to the lower limit, with the upper limit tending to infinity. Generally, for any ordered alloy, the lattice frictional forces are always less than γ (that this may be so can be seen from the fact that the yield strength is less than γ [17] and, hence there are always two limiting equilibrium positions and this fact has to be kept in mind when considering the behaviour of passing dislocations in ordered alloys in comparison with that of disordered alloys.

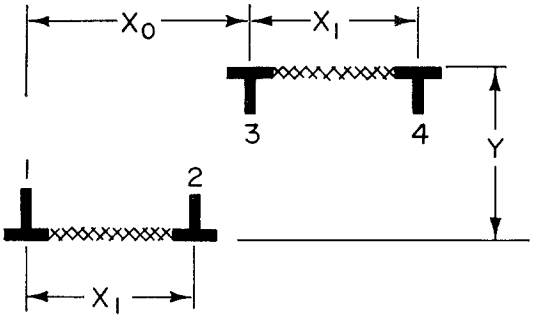


Figure 2 Schematic illustration showing the passage of a pair of superlattice screw dislocations.

3. Passing dislocations

Fig. 2 shows, schematically, the passing of a pair of superlattice screw dislocations. The equilibrium configurations are determined as a function of x_0 by minimizing the total energy of the system. The calculations are similar to that of a disordered alloy except for the contribution from the APB energy to the total energy. The calculations are done first with decreasing x_0 and then with increasing x_0. The calculations are also carried out with x_1 corresponding to the lower limiting equilibrium separation, so that the results can be comparable to those of a disordered alloy [12]. In addition, the calculations are done for infinite straight dislocations and thus are of two-dimensional character.

Fig. 3 shows the variation of x_1 with x_0 for different frictional stresses where the frictional stresses are expressed in units of $[10^{-4}\ \mu m/2\pi]$.

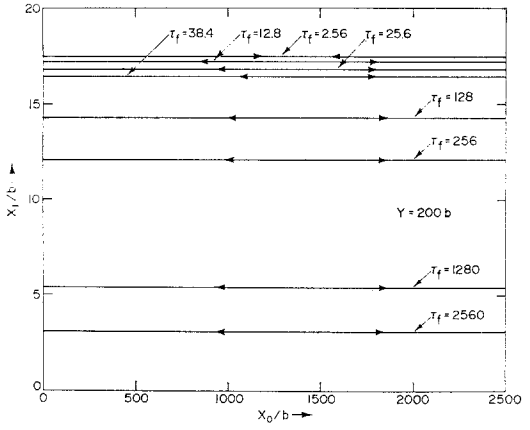


Figure 3 Variation of x_1 with x_0 for a pair of passing superlattice dislocations.

Fig. 3 in particular shows the behaviour of passing dislocations for $y = 200\boldsymbol{b}$, where $\boldsymbol{b}$ is Burgers vector, which is large in comparison with the separation between the partials ($x_1/\boldsymbol{b} = 17.5$, Fig. 1). For a given frictional stress, x_1 remains constant for a complete cycle; i.e., for decreasing and increasing x_0 (Fig. 3). The reason for this behaviour is that the internal stress due to unlike dislocations for such large y is significantly smaller than γ, such that the separation between partials is not affected by passing. On the other hand, equilibrium configurations for the same y, change drastically with decreasing or increasing of x_0 for two pairs of dislocations in a disordered alloy [12] (i.e., when $\gamma = 0$). The decrease of x_1 in Fig. 3 with increasing frictional stress can be understood from Fig. 1, since we considered only the lowering limiting equilibrium for two partials. The force necessary for the dislocations to pass one another can be determined as follows. The total forces acting on dislocation 1 and 2 for increasing x_0 are given by

$$F_1 = F^1{}_I + F^I{}_F - F_a - F_F + \gamma = 0 \quad (1)$$

$$F_2 = F^2{}_I - F^I{}_F - F_a - F_F - \gamma = 0 \quad (2)$$

when $F^i{}_I$ is the force acting on a dislocation i, due to internal stress; i.e., due to the stress field of other dislocations and F_a, F_F and γ are forces due to applied stress, opposing frictional stress, and APB energy, respectively. As explained earlier [12], $F^I{}_F$ is a component of frictional force that is necessary to balance the internal repulsive forces. The force due to applied stress can be determined by combining Equations 1 and 2 to give

$$F_a = -(F_F + (F^1{}_I + F^2{}_I)/2)\,. \quad (3)$$

It is interesting to note that an exactly similar expression was obtained for dislocations in a disordered alloy [12]. Equation 3 may give the impression that the APB energy has no effect on the force necessary for the dislocation to pass. Fig. 3, however, shows that equilibrium configurations are much different due to the presence of γ. Hence, forces $F^1{}_I$ and $F^2{}_I$ will be drastically affected thus γ indirectly contributing to F_a. This contribution can be seen in Fig. 4 where the maximum elastic force; i.e., the maximum force due to internal stress $(F^1{}_I + F^2{}_I)/2$ is plotted as a function of frictional stress.

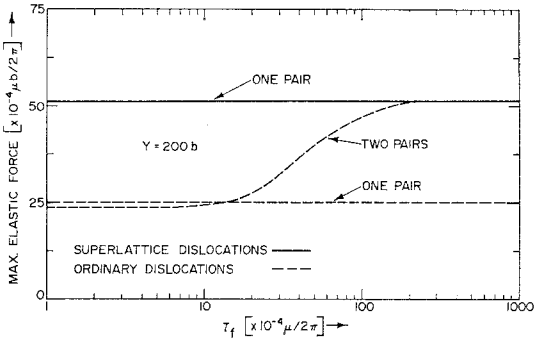
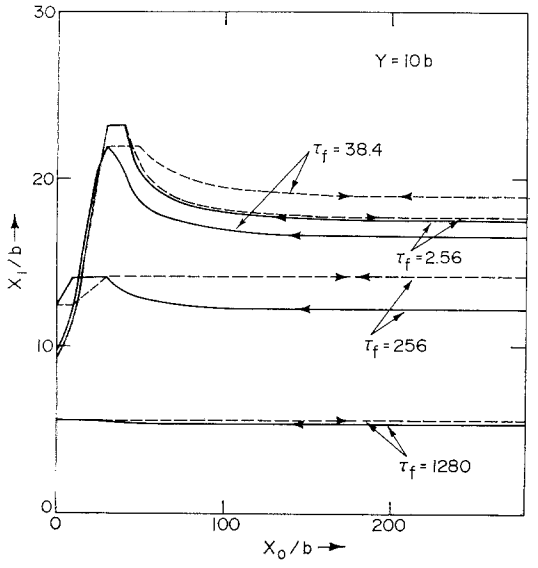
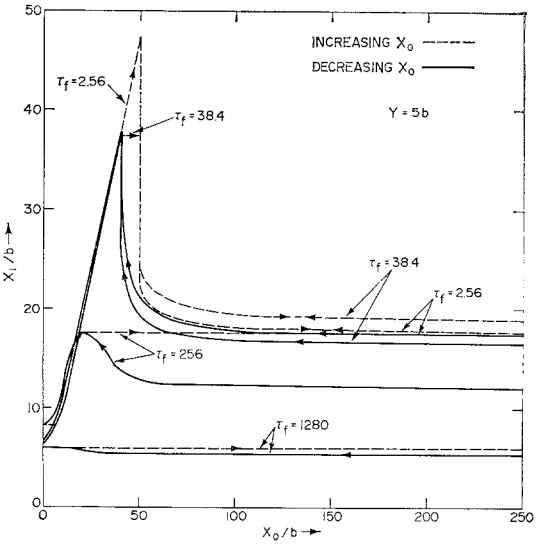


Figure 4 Variation of the maximum elastic force due to internal stress with frictional stress on passing dislocations in ordered and disordered alloys.

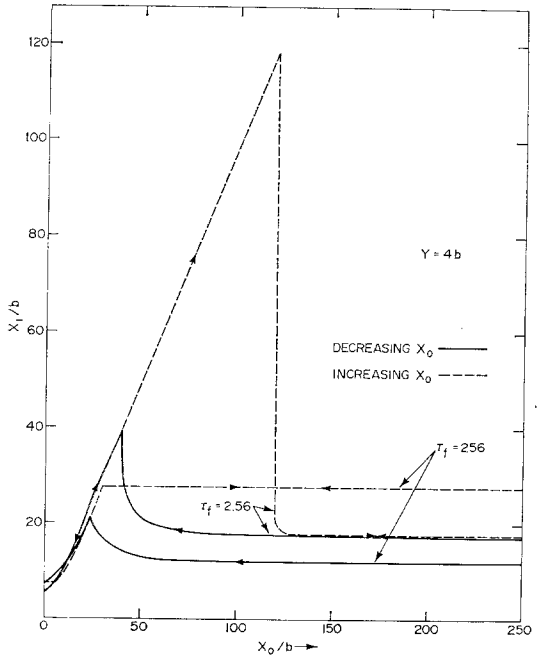
The solid line represents that of the superlattice dislocations while the dotted lines represent that of the ordinary dislocations. Due to the presence of γ, the equilibrium separation, x_1 is much smaller than y. Hence, the dislocations behave as a superdislocation of Burgers vector $2\boldsymbol{b}$ for all ranges of friction. Two pairs of ordinary dislocations also behave as superdislocations of Burgers vector $2\boldsymbol{b}$ at very high frictional forces, provided the dislocations pass one another with minimum separation. Thus, at very high friction forces, the dislocation behaviour is similar in both ordered and disordered alloys. Thus, the above results give a basis for the assumptions made in the previous analysis [13]. At small frictional forces, however, the



(a)



(b)



(c)

Figure 5 (a) (b) and (c) Variation of x_1 with x_0 for a pair of passing superlattice dislocations.

behaviour of a pair of superlattice dislocations is much different from that of two pairs of ordinary dislocations as can be seen in Fig. 4. As the vertical separation decreases, the behaviour of superlattice dislocations even at low frictional stress will be somewhat similar to that of dislocations in a disordered alloy and this is shown below.

Fig. 5a, b and c show, respectively, the equilibrium configurations as a function of x_0 for the vertical separations 10, 5 and 4***b***. From Fig. 1, the vertical separations are smaller than the equilibrium separation of partials at zero frictional stress. These figures show a pronounced variation of x_1 with x_0, especially for small values of x_0. For such values, the internal stresses are much greater than the APB, and hence, x_1 varies drastically with x_0. Furthermore, the above figures show that with an increase of frictional force, the variation in x_1 decreases and the dislocations behave more and more rigidly. For low frictional forces, the configurations for increasing x_0 are much different from those for decreasing x_0. Similar results [10] were observed earlier for zero frictional stress. As x_0 tends to infinity, for frictional stress much less than γ, x_1 tends to two constant values, corresponding to increasing or decreasing x_0, respectively. Further, these two constant values correspond to the two limiting equilibrium values (Fig. 1) and the reason for this is explained below. For decreasing x_0, dislocations are selected at their minimum separation, and hence, x_1 corresponds to the lower limiting equilibrium. For increasing x_0, dislocations 1 and 2 are brought closer after their separation, x_1, has reached some peak value which is much greater than x_{e_2} in Fig. 1. When dislocation 2 swings to dislocation 1, the

equilibrium separation, x_1, then corresponds to the upper limiting equilibrium. However, for frictional forces greater than γ, there is only one limiting equilibrium. In such cases, the equilibrium x_1 in Fig. 5 for increasing x_0 does not correspond to any limiting value. For frictional forces much less than the APB tension the dislocations were found to follow the path given by the dashed line, when x_0 is decreased after one cycle is completed. Also the same (dashed) x_1-x_0 curve is obtained if the dislocations are originally started with decreasing x_0 with x_1 corresponding to the upper limit. This shows that there will be only one set of curves for both decreasing and increasing x_0 for further cycling. Since for frictional stresses less than the APB tension, the equilibrium separation is always restricted between the two limits (Fig. 1), the equilibrium configurations in Fig. 5 are unique functions of x_0 from the second cycle on and they are independent of the initial selection of x_1. For frictional forces greater than γ, however, the path of x_1 sensitively depends on the initial section of x_1 since for such high frictional forces, the upper limiting equilibrium tends to infinity. This behaviour is identical to that of a disordered alloy [12]. For a disordered alloy, there is no unique passing behaviour for all of the frictional stresses and the passing behaviour very much depends on the initial x_1 selected. Fig. 5a, b, and c, show further that with a decrease of y, x_1 increases linearly with x_0 at least at low frictional stresses. Such an increase is associated with the sticking of dislocations [10] 2 and 3 as a dipole while 1 and 4 move apart. Since for such small separations the dipole strength is much greater than γ, splitting of partials occurs in preference to the dipole breaking. As γ tends to zero, the splitting occurs at larger y and in the limit of $\gamma = 0$ corresponding to a disordered alloy, splitting of arrays occurs for all y in the low frictional stress range. In fact, it was observed that dislocations in a disordered alloy [12, 13] cannot pass one another as an array at very low frictional stress. Furthermore, when the frictional stress tends to zero, dislocations in a disordered alloy become completely unstable since they instantly form dipoles and repel one another. The presence of a frictional stress or γ, however, stabilizes these dipoles and dislocations can pass one another as an array. The present analysis, however, only applies to a pair of superlattice dislocations. For large arrays of superlattice dislocations, frictional forces are essential to stabilize them and the analysis of the passing behaviour of large arrays of superlattice dislocations is a subject of further investigation.

It was shown earlier [10] that complete splitting of partials occurs if the vertical separation is below a critical value. For separations greater than the critical values dislocation 2 swings back to dislocation 1 at some x_0, and correspondingly x_1 shows a sharp discontinuity. On the basis of the previous analysis [10] the critical separation y for FeCo was found to be greater than $4\boldsymbol{b}$. Fig. 5c, however, shows that even for $y = 4\boldsymbol{b}$, complete splitting does not occur in FeCo and the shapes of the x_1-x_0 curves for increasing x_0 are much different from those at zero friction [10]. For complete splitting in the presence of frictional forces the internal stress holding dislocations 2 and 3 should be much greater than the sum of frictional stress and APB. Hence, separations much less than $4\boldsymbol{b}$ have to be reached before complete splitting occurs. However, for such very small vertical separations, the cross-slip force will be enormously high and the dislocations can annihilate themselves by non-thermal cross-slip process* which will be discussed later.

Fig. 6 shows the effect of frictional stress on

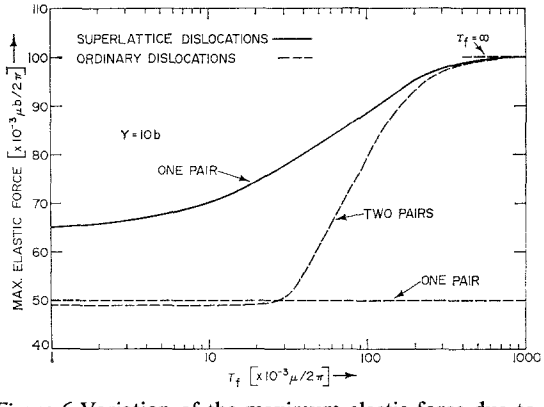


Figure 6 Variation of the maximum elastic force due to internal stress with frictional stress on passing dislocations in ordered and disordered alloys.

*Here we use the term non-thermal process to indicate that a given process can take place without any aid from thermal energy; i.e., even at 0K. This term should not be confused with terms such as athermal process which has been extensively used in the literature to indicate that the contribution from the thermal energy is insignificant in overcoming the given process.

the maximum elastic force on passing dislocations for $y = 10\boldsymbol{b}$. The behaviour of dislocations in a disordered alloy is also represented for comparison. Comparison of Figs. 6 and 4 show that with a decrease of the vertical separation, superlattice dislocations tend to behave as ordinary dislocations. At infinite friction, however, the behaviour of dislocations in both alloys, is identical.

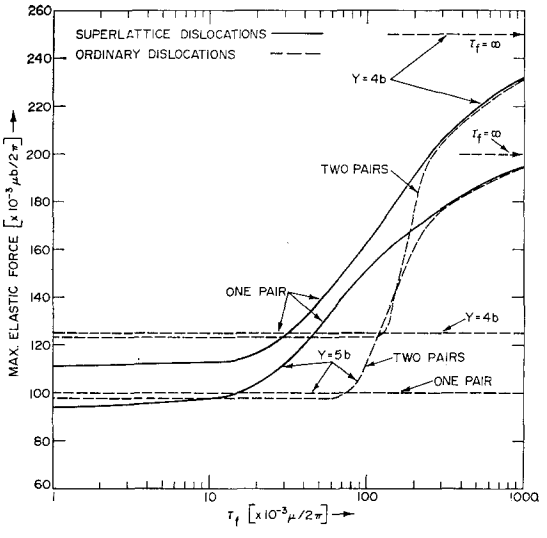


Figure 7 Variation of the maximum elastic force due to internal stress with frictional stress on passing dislocations in ordered and disordered alloys.

The behaviour of superlattice dislocations for $y = 5$ and $4\boldsymbol{b}$ is represented in Fig. 7. Again, the behaviour of ordinary dislocations is represented by dotted lines for comparison. It is interesting to note that at very low frictional stresses the maximum elastic force for one and two pairs of ordinary dislocations is greater than that for a pair of superlattice dislocations. Hence, γ causes weakening instead of strengthening at low frictional stress and low y. The lower elastic force for two pairs of ordinary dislocations, in comparison to that of one pair of ordinary dislocations, was accounted for earlier [13] as due to the contribution from the repulsive force of the inner dipole to the applied stress in breaking the outer dipole. The same reasoning holds good for the case of superlattice dislocations. The maximum force occurs when partials 1 and 3 break away and before the complete splitting occurs. Because of the presence of γ, dislocations 1 and 2 are more closely spaced than when $\gamma = 0$. Hence, the contribution from the repulsive force due to inner dipoles is larger than that in the case of disordered alloys, thus, accounting for the lower elastic force for superlattice dislocations. An essential difference between the superlattice dislocations and the ordinary dislocations, however, is that superlattice dislocations pass as an array despite some amount of stacking, while for disordered alloys, dislocations split from the array for all vertical separations. Dislocation splitting in ordered alloys may be observed for very small y at low frictional stresses.

It is next of interest to study the variation of the maximum elastic force as a function of y at a constant frictional stress. This is represented in Fig. 8 when the maximum elastic force is plotted as a function of log (y/b). Calculations are done at a constant friction stress, $\tau_f = 45$, corresponding to the yield stress of an ordered FeCo alloy [17] and the magnitude of τ_f is much smaller than γ, the APB energy. Fig. 8 shows that except at very small y, the maximum elastic force for superlattice dislocations is greater than that for ordinary dislocations. At large y, similar to the case at large friction, the behaviour of ordinary dislocations and superlattice dislocations is identical. At very small y, however, the maximum elastic force for superlattice dislocations is less than that of ordinary dislocations and

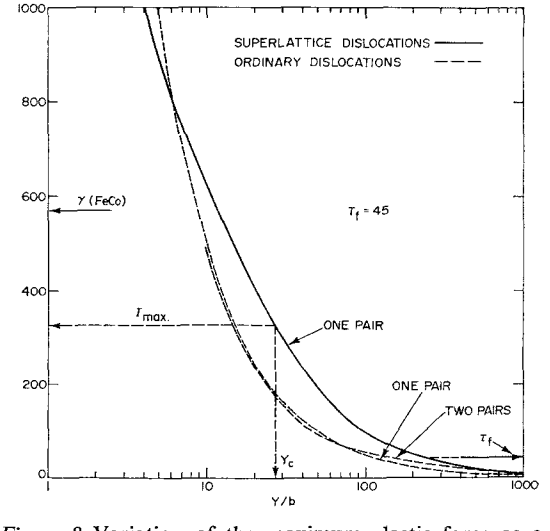


Figure 8 Variation of the maximum elastic force as a function of y for passing dislocations in ordered and disordered alloys.

the reason for this lower force has been accounted for earlier.

It was also argued earlier [13] that high work-hardening in ordered alloys arises due to two factors; an increased dipole strength and a reduced cross-slip activity. Since the frictional stress is very small in comparison with a dipole strength, the strengthening by increasing the number of passing superlattice dislocations is possible only at large y [13]. At smaller y, less than $250\boldsymbol{b}$; i.e., when the dipole strength of a superlattice dislocation is greater than τ_f, the passing stress is essentially controlled by the dipole strength (Fig. 8). However, as y decreases, corresponding to an increase in strain, the density of cross-slip sites also increases.

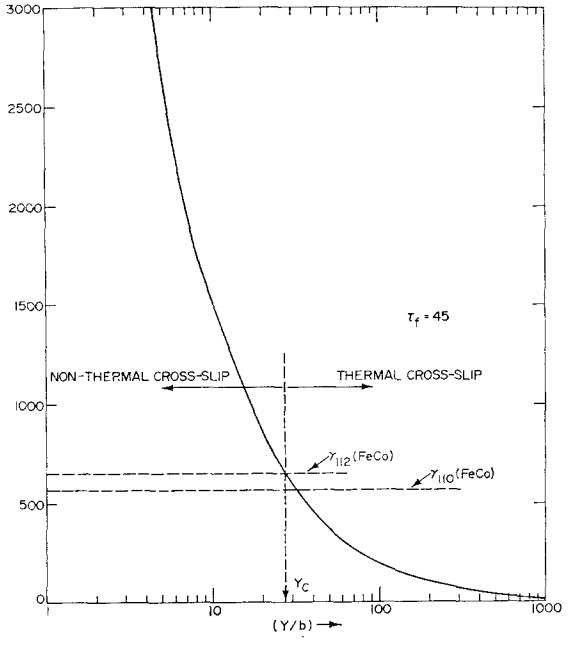


Figure 9 Variation of the maximum cross-slip force on superlattice dislocations as a function of y.

Fig. 9 shows the variation of the maximum cross-slip force for a superlattice dislocation as a function of y. It is important to notice that the cross-slip force at a given y is nearly two times greater than the corresponding maximum elastic force on the slip plane (Fig. 8). The value of γ_{110} and γ_{112} of FeCo is also represented in Fig. 8. If $\{110\}$ is a slip plane and $\{112\}$ a cross-slip plane, superlattice dislocations are able to cross-slip non-thermally if the vertical separation is less than y_c (Fig. 9) where the cross-slip force for y less than y_c is greater than γ_{APB}.

The cross-slip on planes other than $\{112\}$ could also be considered. In such cases the component of cross-slip force (Fig. 9) on the given plane has to be equated to the corresponding APB on that plane to determine y_c. From Fig. 8 the maximum elastic force on the slip plane for $y = y_c$ is represented by τ_{max}. The significance of τ_{max} in Fig. 8 is that it represents the maximum strengthening that can be obtained by passing superlattice screw dislocations. If the vertical spacing is less than or equal to y_c, a spontaneous cross-slip occurs leading to annihilation of passing dislocations. This spontaneous cross-slip will be referred to as non-thermal cross-slip since for $y \leqslant y_c$, there may not be a thermal energy barrier for cross-slip. For y greater than y_c, however, cross-slip could be thermally activated with internal stress (cross-slip force) aiding the activation process. Since the contribution to the activation energy from the cross-slip force due to internal stress is a function of y, it follows that the activation energy for cross-slip should be a function of y, or in turn, should be a function of strain. Since a decrease in y is related to an increase in strain the activation energy for cross-slip should decrease with the increase in strain. Also, τ_{max} in Fig. 8 is nearly half of γ_{APB} implying that screw dislocations will annihilate themselves before they can split giving rise to full APB. Also, cross-slip could take place on planes belonging to $\langle 111 \rangle$ zone even without constricting into a perfect dislocation as in Schoeck and Seeger's model [18]. Instead, the leading partials can cross-slip independently with the aid of the internal stress, while the APB tension pulls the other partial with it. Consistent with the above arguments is the fact that with an increase of γ (APB), σ_{III}, corresponding to the onset of stage III, increases [17] and this is contrary to that expected from the constriction model. Figs. 8 and 9, however, show that with an increase of γ, y_c decreases and, hence, τ_{max} increases implying that larger stresses are reached before non-thermal cross-slip takes place. The same conclusion holds good for thermal cross-slip, implying that higher internal stresses are needed before cross-slip can be thermally activated, thus accounting for the increase of σ_{III} with γ. However, if γ is very high as in β-brass [19], the partials in a superlattice dislocation are so close that Seeger's

constriction model may be applicable for cross-slip. In such cases, the cross-slip force due to internal stress will be effective after the constriction has taken place.

The analysis thus far applies only to passing screw dislocations. It was shown earlier that the passing behaviour of edge dislocations is somewhat similar to that of screw dislocation but more complicated [10]. Even for edge dislocations, the dipole strength increases with a decrease of y. Unlike the case for screw dislocations, however, non-thermal recovery leading to annihilation is very difficult for edge dislocations. Though climb force due to internal stresses on edge dislocations increases with decrease of y, stresses of the order of theoretical elastic limit have to be reached before non-thermal climb can occur, since it involves the creation of point defects [20]. For ordered alloys, the energy needed for climb will be much more since it involves the creation of non-shear antiphase boundaries [21]. The suppression of climb processes for passing edge dislocation implys that very small values of y can be reached with increasing strain, and for such small y values, splitting of partials can occur in preference to dipole breaking. At this stage, it is not quite clear what the relative contributions from passing screw and edge dislocations to the total work-hardening in ordered alloys is, and this has to await further study.

As mentioned earlier only infinite straight dislocations are considered in the present calculations. The passing dislocations could also have kinks along their length, however, the passing stress may not be affected to any significant extent since the kinks have no long range stress fields [21]. The passing stress may be affected by the presence of kinks if the separation between the passing dislocations is comparable to the spacing of the kinks. On the other hand, when the separation between the passing dislocations is that small, there will be large internal stresses on each dislocation and the equilibrium configuration of the kinks in the presence of such high internal stresses is not yet understood. Furthermore, the infinite dislocation approximation may not be a realistic description in such a situation.

4. Summary and conclusions

A detailed analysis of the behaviour of passing superlattice screw dislocations is presented and the results are compared with that of ordinary dislocations. In particular, it was shown that the behaviour of superlattice dislocations is similar to that of ordinary dislocations at very high frictional stresses, as well as at very low vertical separations. However, with the decrease of y, or in turn, with the increase of strain, the cross-slip force on passing dislocations also increases to an extent that non-thermal cross-slip can occur annihilating the passing dislocations. Thus, the stress induced recovery will set a limit for the maximum work-hardening that can be reached by passing screw dislocations. On the other hand, such annihilation is practically impossible for passing edge dislocations since it involves climb processes. Hence, the vertical separation, y, can decrease with strain for passing edge dislocations to a limit where splitting of superlattice dislocations can occur in preference to dipole breaking. Although the above calculations were done specifically for the FeCo alloys, the results of this analysis are quite general and should be applicable to all B2 alloys. Also, the calculations have considered the frictional stress as a phenomological constant and was associated with lattice frictional forces. The analysis, however, can be more general since it is valid for any type of frictional forces that offer resistance to the motion of dislocations. For example, frictional forces could be drag forces induced by jogs on the passing dislocations and in such cases the magnitude of the frictional force could be a function of strain.

Acknowledgements

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