

DISLOCATION ARRANGEMENTS IN TANTALUM SINGLE CRYSTALS DEFORMED IN TENSION AT 373°K*

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The dislocation structure in tantalum single crystals deformed in tension to various strains at 373°K has been investigated by transmission electron microscopy. Foils were prepared by a disc technique and various sections were analyzed at each strain. In stage I of the stress-strain curve tangles of dislocations are observed lying parallel to the slip plane; these tangles contain many straight screw dislocations and a high density of dislocation loops. In stage II the tangles tend to become linked together to form walls of dislocations approximately parallel to the slip plane. Misorientations across the walls become increasingly apparent as the crystals are deformed further into stage II and stage III. It is suggested that the walls are small-angle boundaries formed when short-range secondary slip occurs to reduce the long-range stresses at the ends of slip lines. Accordingly a high density of secondary dislocations is observed. The flow stress is found to be proportional to the square root of the total dislocation density.

Dislocation reactions in b.c.c. metals are analyzed and a quantitative theory of stage II hardening is developed based on the cell formation theory of Hirsch.

ARRANGEMENTS DE DISLOCATIONS DANS DES MONOCRISTAUX DE TANTALE DEFORMES PAR TRACTION A 373°K

Les auteurs ont étudié en microscopie électronique par transmission la structure des dislocations dans des monocristaux de tantale déformés par traction jusqu'à diverses déformations à 373°K. Les lames métalliques minces sont préparées par une technique de disque et plusieurs échantillons sont analysés pour chaque déformation. Dans le stade I de la courbe tension-déformation, on observe des écheveaux de dislocations situés parallèlement au plan de glissement; ces écheveaux contiennent beaucoup de dislocations-vis rectilignes et une grande densité de boucles de dislocations. Dans le stade II, les écheveaux tendent à se réunir pour former des frontières de dislocations approximativement parallèles au plan de glissement. Des désorientations au travers des frontières sont de plus en plus apparentes lorsque les cristaux sont déformés plus avant dans le stade II et le stade III. Les auteurs suggèrent que les frontières sont des frontières à petits angles formées lorsque le glissement secondaire à courte distance apparaît pour réduire les tensions à longue distance aux extrémités des lignes de glissement. En conséquence, on observe une haute densité de dislocations secondaires. La limite élastique est proportionnelle à la racine carrée de la densité totale de dislocations.

Les auteurs analysent les réactions de dislocations dans les métaux corps centrés et développent une théorie quantitative du stade II du durcissement basée sur la théorie de Hirsch de formation de cellules.

VERSETZUNGSANORDNUNGEN IN TANTALEINKRISTALLEN NACH ZUGVERFORMUNG BEI 373°K

Die Versetzungsstruktur von bei 373°K zugverformten Tantaleinkristallen wurde für verschiedene Verformungsgrade im Elektronenmikroskop untersucht. Die dünnen Folien wurden mit Hilfe eines Scheibenverfahrens hergestellt. Bei jedem Verformungsgrad wurden mehrere Schnitte untersucht. Im Bereich I der Verfestigungskurve beobachtet man Versetzungsstränge parallel zur Gleitebene. Diese Stränge enthalten zahlreiche gerade Schraubenversetzungen und eine hohe Dichte von Versetzungsringen. Im Bereich II tendieren die Stränge zur Verbindung untereinander unter Bildung von Versetzungswänden etwa parallel zur Gleitebene. Fehlorientierungen über die Wände hinweg erscheinen in zunehmendem Maße bei weiterer Verformung der Kristalle in den Bereichen II und III. Bei den Wänden handelt es sich vermutlich um Kleinwinkelgrenzen, die sich bilden, wenn eine kurzreichende Sekundär-gleitung zur Verminderung der weitreichenden Spannungsfelder an den Enden von Gleitlinien auftritt. Entsprechend wird eine hohe Dichte von Sekundärversetzungen beobachtet. Die Fließspannung erweist sich als proportional zur Quadratwurzel aus der gesamten Versetzungsdichte.

Die Versetzungsreaktionen in k.r.z. Metallen werden analysiert. Aufbauend auf die Zellbildungs-theorie von Hirsch wird eine quantitative Theorie der Verfestigung im Bereich II entwickelt.

1. INTRODUCTION

Recent work on the deformation behavior of single crystals of tantalum deformed in tension has shown that three-stage hardening is observed over a range of orientations, temperatures and strain-rates.^(1,2) This is in accord with other recent work on b.c.c. crystals of niobium^(3,4) and iron⁽⁵⁾ where three-stage hardening

is also observed. Therefore, it appears that three-stage hardening is a general phenomenon in b.c.c. metals just as in f.c.c. metals. Additional recent work on single crystal deformation has shown that three-stage hardening is also observed in close packed hexagonal metals (zinc,⁽⁶⁾ cadmium,⁽⁷⁾ cobalt⁽⁸⁾ and magnesium⁽⁹⁾), in germanium and indium antimonide,⁽¹⁰⁾ and in sodium chloride.⁽¹¹⁾ Therefore, it seems likely that when three-stage hardening does occur in materials with different structures there should be a common dislocation model applicable to

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each. That is, although the dislocation interactions involved vary with the crystal structure the basic hardening mechanism should be similar.

The present paper describes the results of a transmission electron microscopy analysis on tantalum single crystals deformed in tension at 373°K and examined throughout three-stage hardening. The dislocation substructures observed are discussed in relation to work-hardening in b.c.c. metals.

2. EXPERIMENTAL TECHNIQUES

The techniques used to grow, prepare and deform the tantalum single crystals have been described previously.^(1,2) The only orientation investigated was one near the middle of the stereographic triangle where three-stage hardening was prominent. The crystals were deformed at 373°K using a strain-rate of $9.3 \times 10^{-4} \text{ sec}^{-1}$. The tensile specimens were 4.5 cm long with a gage length of 2.5 cm and a gage diameter of 3.0 mm. Specimens suitable for transmission electron microscopy were prepared from tensile specimens deformed to various strains in the following way. Discs approximately 1.5 mm thick were cut from the cylindrical tensile specimens using a spark wire-cutter. The thickness was then reduced to approximately 0.7 mm by spark-planing both sides of the disc an equivalent amount. The final electropolishing operation was performed in a solution of 90 parts sulphuric acid and 10 parts hydrofluoric acid using a teflon holder⁽²⁾ similar to that described by Briers *et al.*⁽¹²⁾ Polishing was stopped when a hole first appeared in the disc, as detected by transparency to light. The region around the hole was found to be suitable for examination in a JEM-6A electron microscope operating at 100 kV. Thin foils were prepared from discs cut perpendicular to the tensile axis and parallel to the (011) plane (approximately the slip plane). In one case an additional foil was prepared from a section perpendicular to the primary slip direction [111].

3. EXPERIMENTAL RESULTS

Dislocation substructures were observed in tantalum crystals deformed at 373°K ($\dot{\epsilon} = 9.3 \times 10^{-4} \text{ sec}^{-1}$) in all three work-hardening stages at shear strains of $\epsilon = 0.03, 0.08, 0.15, 0.35, 0.45, 0.63$ and 0.76. The appropriate shear stress-shear strain curve and the orientation of the crystals is shown in Fig. 1. For this orientation in the standard stereographic triangle [001]-[101]-[111], the primary slip direction was [111] and the primary slip plane was found to be approximately the maximum resolved shear stress plane which is about 6 degrees from (011).⁽¹⁾ With this nomenclature, the secondary

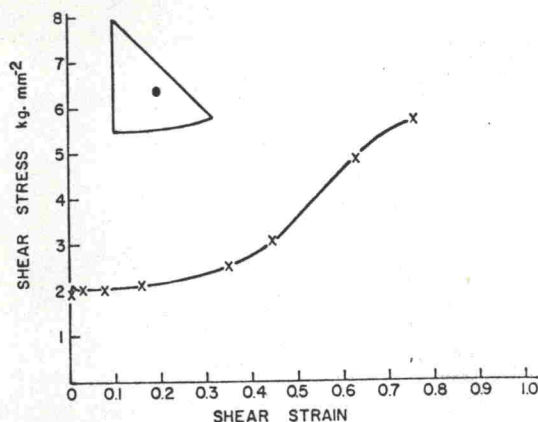


FIG. 1. Typical shear stress-shear strain curve of tantalum single crystals used for transmission electron microscopy, showing strains at which sections were examined (X), ($T = 373^\circ\text{K}$, $\dot{\epsilon} = 9.3 \times 10^{-4} \text{ sec}^{-1}$).

dislocations have Burgers' vectors parallel to [111], [111] and [111]; the last may also be called the conjugate slip direction since it operates in double slip at the [001]-[101] symmetry boundary. In the transmission electron micrographs given in the following sections, the reciprocal lattice vector, g , of the predominant reflection is indicated using the same nomenclature.

The reliability of the experimental techniques used to prepare thin foils was tested by looking at an undeformed crystal. Practically no dislocations were found in specimens made from sections perpendicular to the growth axis of the rods of as-grown crystals. This was good evidence that the procedure used in the preparation of the thin films was such that any damage introduced into the specimens during spark-cutting and spark-planing was removed during the subsequent electropolishing treatment. Specimens strained to about 1% (prior to yielding) showed a slight increase in dislocation density; however, only a few dislocation interactions were observed and the dislocation distribution was non-uniform.

The dislocation structures observed in each stage of deformation are described below.

3.1 Dislocation distribution in stage I

Specimens strained to 3% (just beyond yielding) showed a considerable increase in dislocation density and numerous interactions between primary and secondary dislocations could be observed. Sections parallel to the (011) plane showed many nearly straight dislocations parallel to the $\langle 111 \rangle$ directions (see Fig. 2). Contrast experiments revealed that these are in fact screw dislocations with Burgers vectors parallel to [111] (the primary slip direction) and [111] (a secondary slip direction). It was estimated

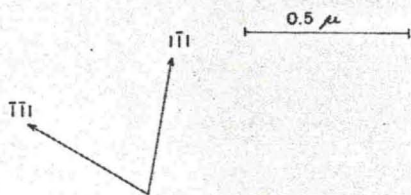
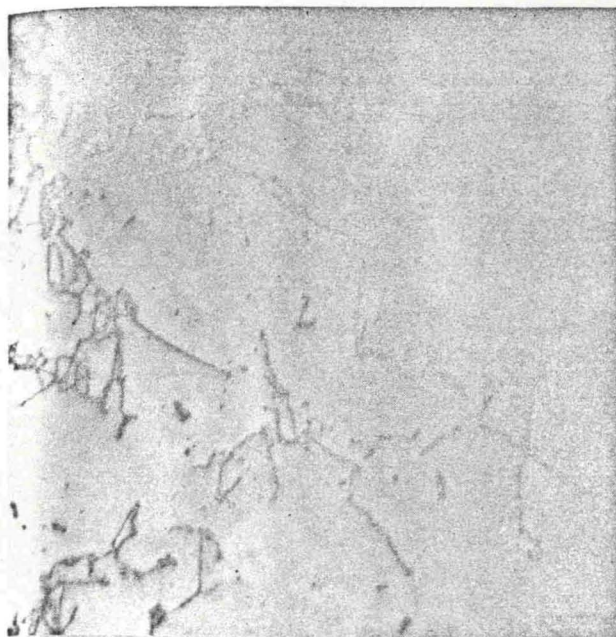


Fig. 2. Beginning of stage I, $\epsilon = 0.03$, section parallel to (011), $g = (200)$. Most of the dislocations lie parallel to $\langle 111 \rangle$ directions and are screw dislocations.

from Fig. 2 and similar micrographs that the primary dislocation density is about twice as great as the secondary dislocation density. However, the other two types of secondary dislocations may also be present in quantity, but they cannot easily be detected in (011) sections. It can still be concluded that there are a considerable number of secondary dislocations already present at this early stage of deformation. Dislocations or dipoles with edge character are almost entirely absent, in contrast to f.c.c. metals.⁽¹⁴⁾ However, Fig. 2 shows that there is a considerable number of nearly circular dislocation loops present along with various other debris, much of which may be small loops which cannot be resolved. In sections perpendicular to the tensile axis the dislocation segments were observed to be short, as is to be expected if they are screw dislocations at a large angle to the foil surface, and there was a tendency for dislocations to occur in tangles parallel to the trace of the primary slip plane.

The dislocation distributions after 8% strain were found to be much the same as those present after 3%

strain. However, the dislocations showed a greater degree of interaction and the resultant tangle appeared to be lined up along the primary slip plane. Figure 3 is representative of sections parallel to the (011) plane and it shows long dislocations parallel to the $[111]$ primary slip direction and shorter segments parallel to the $[\bar{1}\bar{1}1]$ direction. These are again screw dislocations.

For specimens strained to 15%, sections perpendicular to the tensile axis (Fig. 4) show a definite alignment of dislocation tangles parallel to the trace of the maximum resolved shear stress plane (MRSSP). In between the tangles the dislocation density is fairly low. Sections parallel to the (011) plane (Fig. 5) show a considerably different distribution from those perpendicular to the tensile axis. As seen in Fig. 5 the dislocation distribution in (011) sections is more uniform. This is to be expected if the tangles are nearly parallel to the (011) planes as indicated previously. There is still a marked tendency for dislocations to lie parallel to $\langle 111 \rangle$ directions. A micrograph from a third type of foil, normal to the

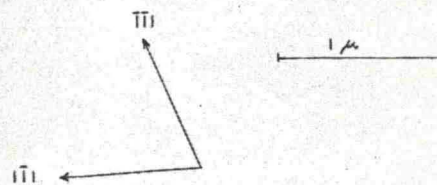
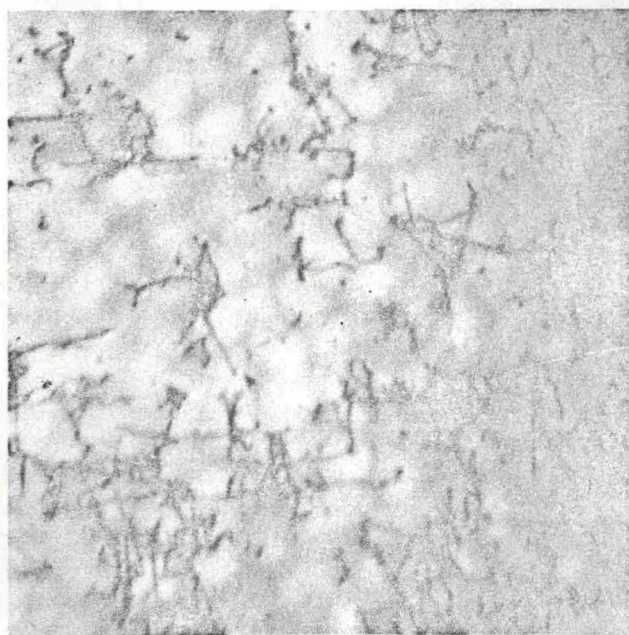


Fig. 3. Early in stage I, $\epsilon = 0.08$, section parallel to (011), $g = (0\bar{1}1)$, $(2\bar{1}\bar{1})$. Most of the dislocations still lie along screw directions.

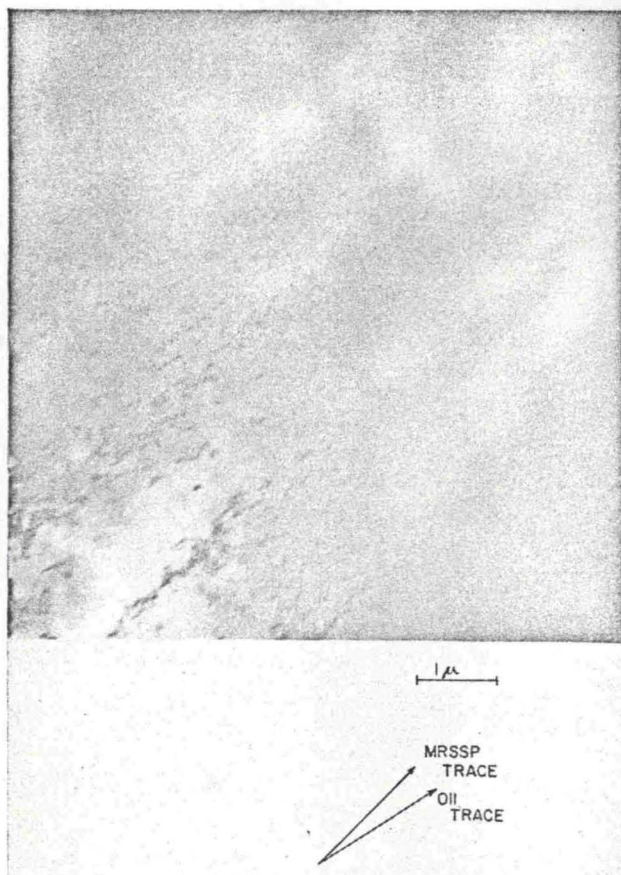


FIG. 4. Middle of stage I, $\epsilon = 0.15$, section normal to tensile axis, $g = (1\bar{2}1)$. The tangles lie parallel to the trace of the primary slip plane.

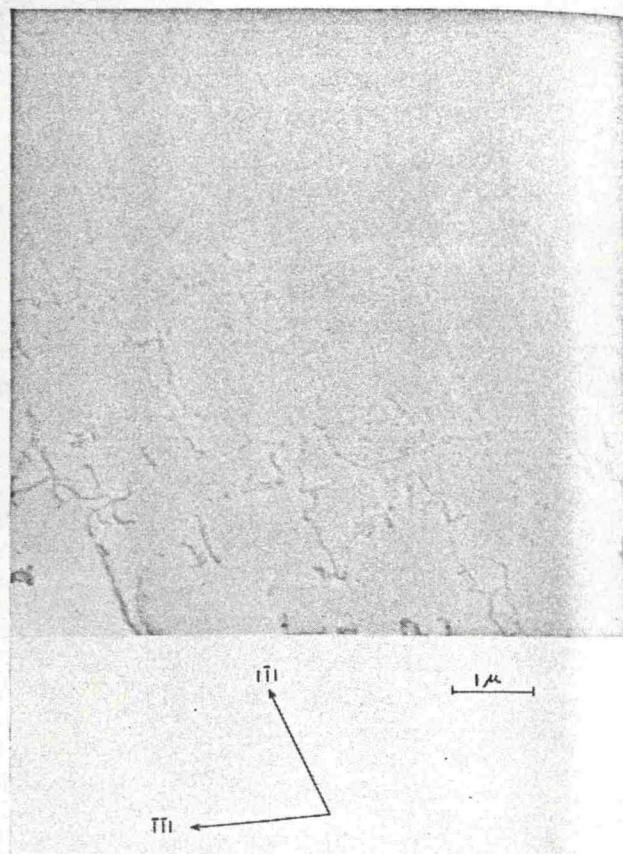


FIG. 5. Middle of stage I, $\epsilon = 0.15$, section parallel to (011) , $g = (011)$. Dislocations still lie along screw directions.

primary slip direction $[1\bar{1}1]$ is shown in Fig. 6. This shows clearly the tangles parallel to the primary slip plane; the tangles presumably contain the $[1\bar{1}1]$ primary dislocations and the $[111]$ secondary dislocations. Figure 6 also shows that there are many dislocation segments linking the tangles; most of these dislocations lie parallel to projections of either the $[111]$ or $[1\bar{1}1]$ directions and it is likely that they are secondary screw dislocations. Contrast experiments established that all three types of secondary dislocations were present in the micrographs.

3.2 Dislocation distribution at the transition from stage I to stage II

These specimens were deformed to a shear strain of about 35%. Figure 7 shows that in sections perpendicular to the tensile axis there is still a tendency for tangles to lie parallel to (011) or maximum resolved shear stress traces. However, the tangles are much broader and appear to be joining up in an irregular manner. Numerous dislocation loops are still evident and it appears that many of the loops are more

elongated than those observed previously. It is also apparent that high concentrations of dislocation loops are associated with the tangles. In sections parallel to the (011) plane there is still some tendency for dislocations to be screwy but long segments of screw dislocations are rarer.

3.3 Dislocation distribution in stage II

For specimens strained about 45% to the beginning of stage II, sections normal to the tensile axis (Fig. 8) show the beginnings of the formation of an elongated cell structure. In Fig. 8 the light and dark contrast across adjacent boundaries is clearly evident. These boundaries or cell walls probably form from the joining up of dislocation tangles. The alternating black and white contrast in Fig. 8 is due to misorientations developing across the walls of dislocations parallel to the primary slip plane. It is apparent that small-angle boundaries are being formed. Surface relaxation effects due to screw dislocations in the cell walls showed that alternate walls contained forest dislocations of opposite sign.⁽¹³⁾ This has also been

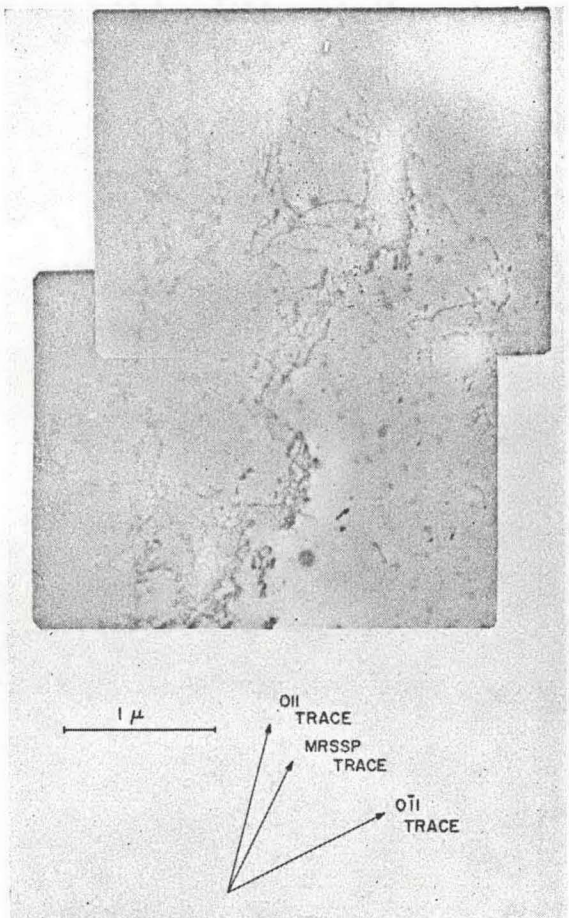


FIG. 7. Transition from stage I to stage II, $\epsilon = 0.35$, section normal to the tensile axis, $g = (020)$. The dislocation tangles have thickened and have become linked together by secondary slip.

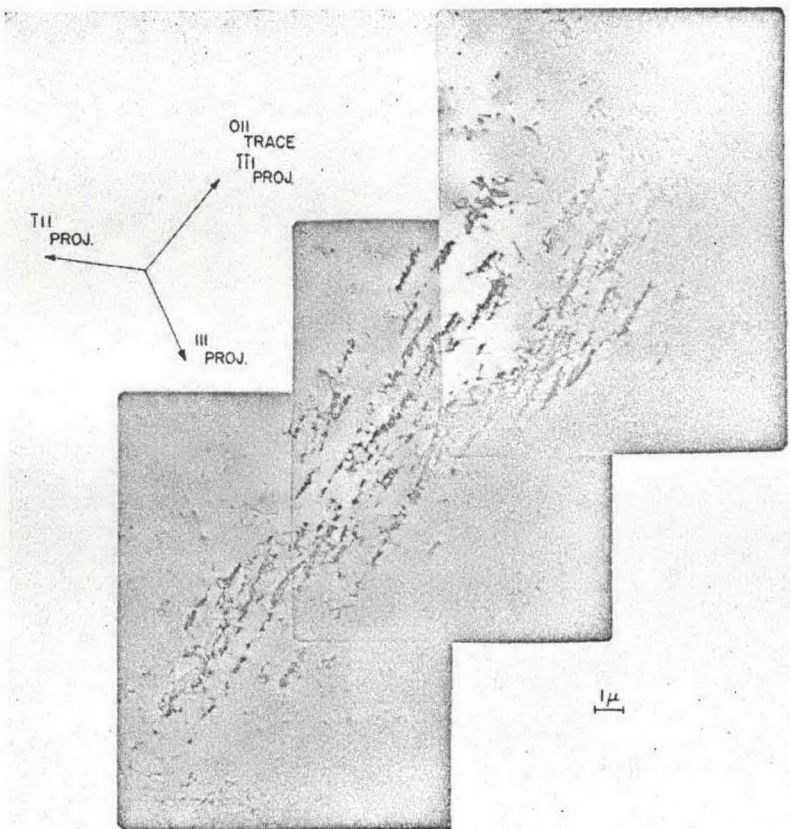


FIG. 6. Middle of stage I, $\epsilon = 0.15$, section normal to $[111]$ primary slip direction, $g = (011)$. The tangles lie parallel to the trace of the primary slip plane. The dislocations between the tangles are secondary dislocations.

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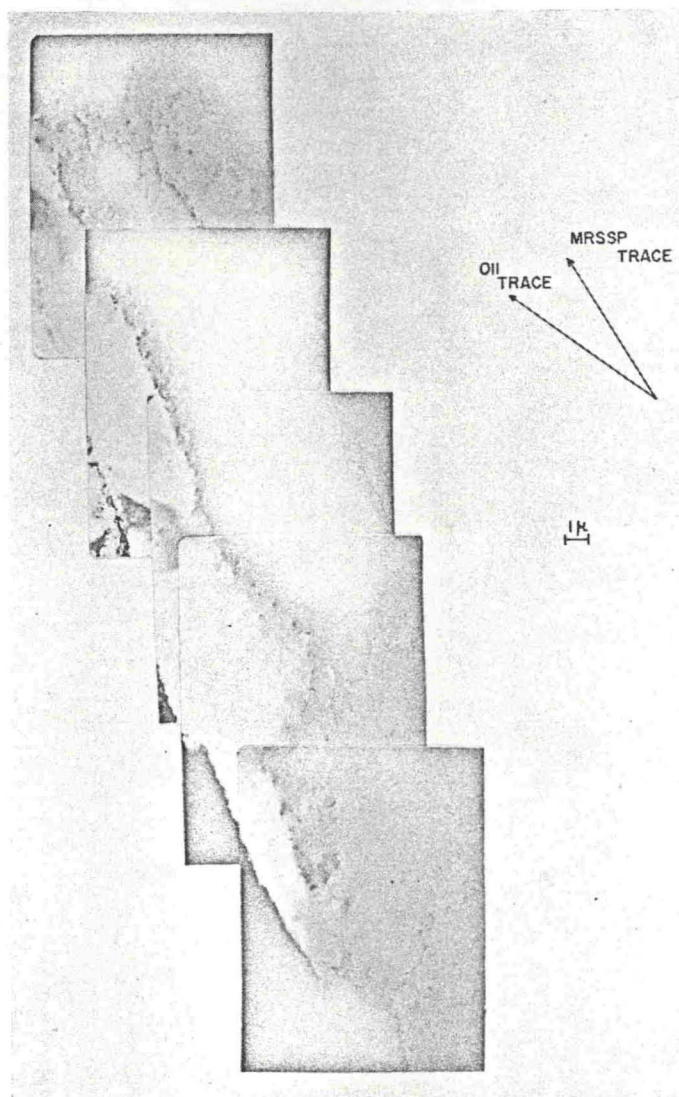


FIG. 8. Beginning of stage II, $\epsilon = 0.45$, section normal to tensile axis, $g = (\bar{2}11)$. The black and white contrast across dislocation walls is due to misorientations. The walls lie parallel to the trace of the primary slip plane.

observed in copper⁽¹⁴⁾ and it is suggested that the separation of these walls is a measure of the secondary slip distance, which is thus much smaller than the primary slip distance. Figure 9 shows that a network structure is starting to form in the (011) plane and also that while dislocations still tend to lie along $\langle 111 \rangle$ directions many of them lie in other directions. There appear to be numerous dislocations in the network that lie in the vicinity of the [100] direction. As shown in Section 4, reactions between primary and secondary dislocations can produce $a\langle 001 \rangle$ dislocations lying in $\langle 100 \rangle$ directions; however, contrast experiments have not yet established the existence of such reaction products with any certainty. Figure 9 and other micrographs show that there is

also a tendency for dense dislocation regions to lie parallel to $[1\bar{1}1]$, $[11\bar{1}]$ and $[100]$ directions, which are lines of intersection of $\{110\}$ secondary slip planes with the primary (011) plane. Hence the dense dislocation regions in the primary slip plane may be due to secondary slip on $\{110\}$ planes interfering with primary slip.

Near the end of stage II (63% strain) the greater contrast between adjacent cells in sections normal to the tensile axis indicates that the misorientation between cells has increased (Fig. 10). Kikuchi line analysis of selected area diffraction patterns showed that the misorientations across the cell walls are $\sim \frac{1}{2}^\circ$. At this stage the cell walls do not appear to line up very regularly along either the (011) or

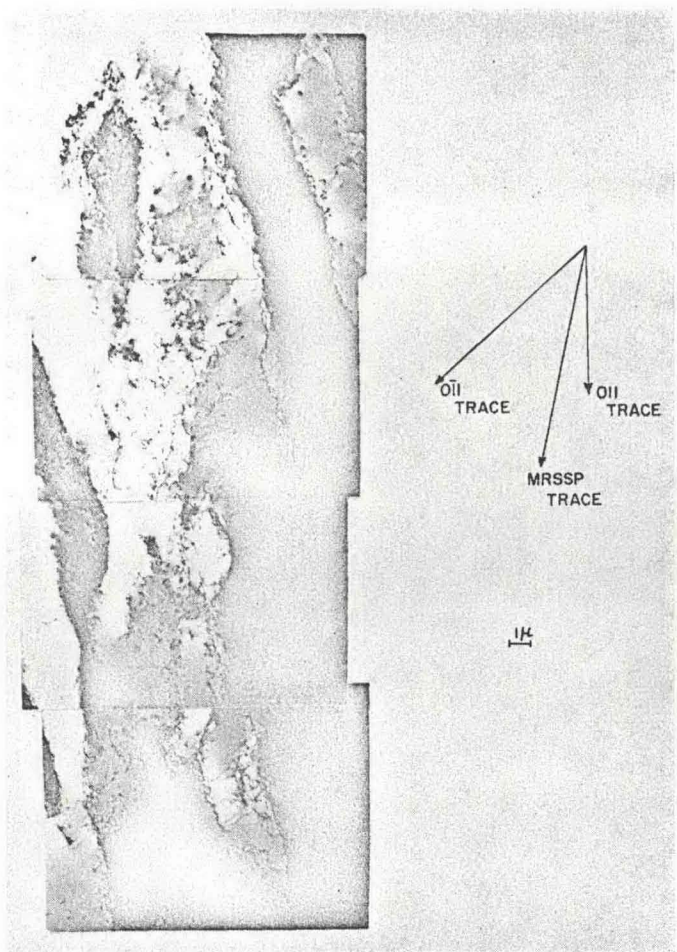


FIG. 10. Stage II, $\epsilon = 0.63$, section normal to tensile axis, $g = (211)$, $(2\bar{1}\bar{1})$. The elongated cell structure is becoming highly developed with alternate misorientations across dislocation walls.

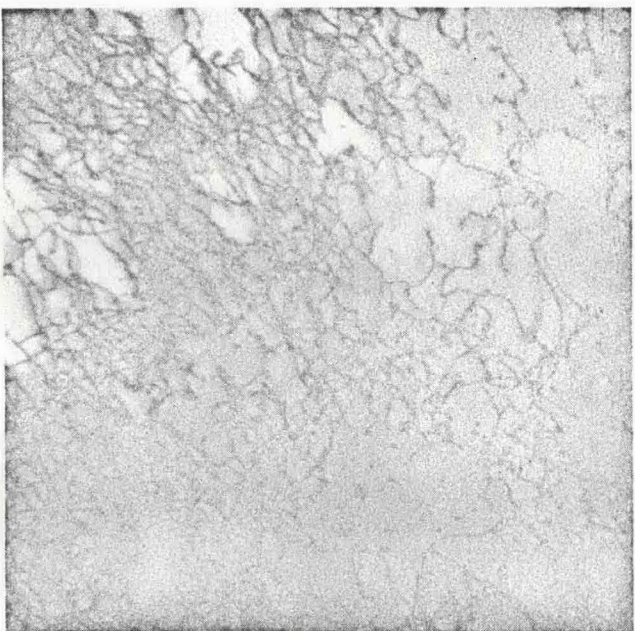


FIG. 9. Beginning of stage II, $\epsilon = 0.45$, section parallel to (011) , $g = (200)$. Dislocations still lie along $\langle 111 \rangle$ directions but there are also dislocations lying in the $[100]$ direction. A network structure is starting to form in the (011) plane.

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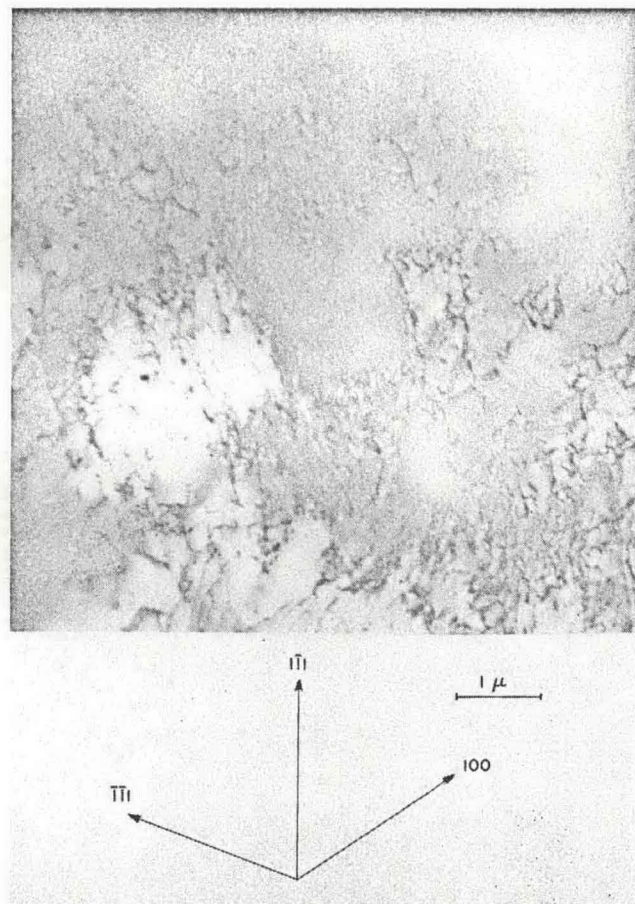


FIG. 11. Stage II, $\epsilon = 0.63$, section parallel to (011) , $g = (2\bar{1}1)$. Note the tendency for dense regions of dislocations to lie parallel to $[100]$ and $\langle 111 \rangle$ directions, which are lines of intersection with secondary $\{110\}$ planes.

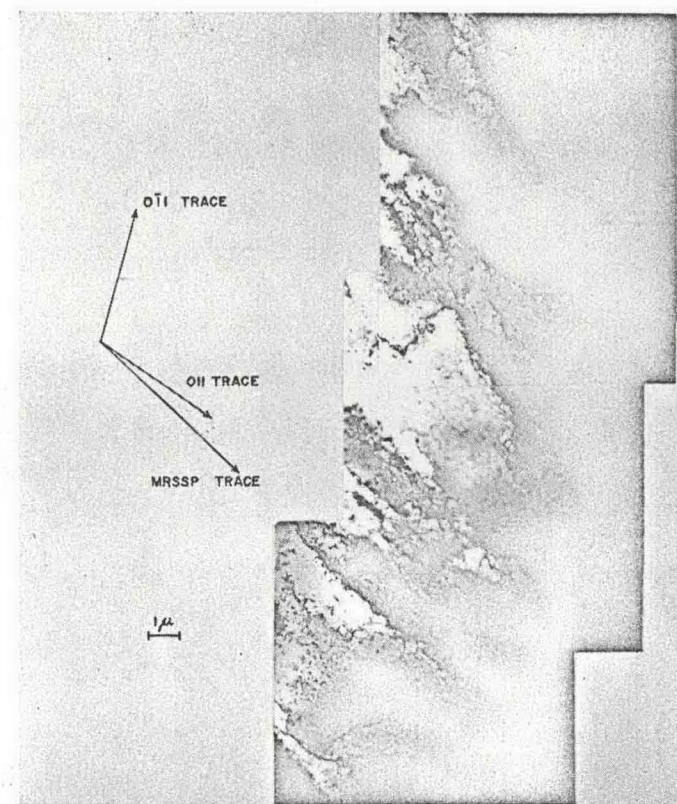


FIG. 12. Stage III, $\epsilon = 0.76$, section normal to tensile axis, $g = (\bar{1}\bar{2}1)$. The cell structure is more non-uniform than previously as a result of secondary slip producing cells that are more equiaxed.

maximum resolved shear stress traces. Sections parallel to the (011) plane (Fig. 11) show that dislocations still line up along $\langle 111 \rangle$ directions and a network structure is present which appears to be in a more advanced state than that observed on similar sections after 45% strain. There is no black and white contrast in sections parallel to the (011) plane since the walls of dislocations (which are small angle boundaries) lie approximately in this plane. Since the misorientations across the wall were only analyzed in one type of section (perpendicular to the tensile axis), the nature of the boundaries could not be established with certainty. However, Kikuchi line analysis of this section (e.g. Fig. 10) was consistent with most of the cell walls being within 30° of pure tilt boundaries.

3.4 Dislocation distribution in stage III

The specimens examined in this stage were deformed to a shear strain of 76%. At this strain the conjugate slip system also has a high shear stress acting on it.

Figure 12 shows the predominant cell structure that is evident in sections perpendicular to the tensile axis. There appear to be regions adjacent to cell boundaries where considerable secondary slip has occurred producing cells that are more equiaxed. This results in the appearance of a more non-uniform cell structure than that observed previously. Cell walls are also observed to lie along the $(0\bar{1}1)$ trace which is the trace of the conjugate slip plane. Sections parallel to the (011) plane showed two different types of structure. A network structure similar to that observed after 63% strain was formed over about half of the foil (Fig. 13) but an elongated cell structure showing black and white contrast (Fig. 14) was also present. The black and white contrast apparent in the (011) plane probably arises from the $(a/2)[111]$ secondary dislocations which have a large resolved shear stress acting on them at this stage and consequently are able to move over large distances. These dislocations are then able to produce dislocation

Fig. 11. Stage II, $\epsilon = 0.63$, section parallel to (011), $g = (2\bar{1}1)$. Note the tendency for dense regions of dislocations to lie parallel to $[100]$ and $\langle 111 \rangle$ directions, which are lines of intersection with secondary $\{110\}$ planes.

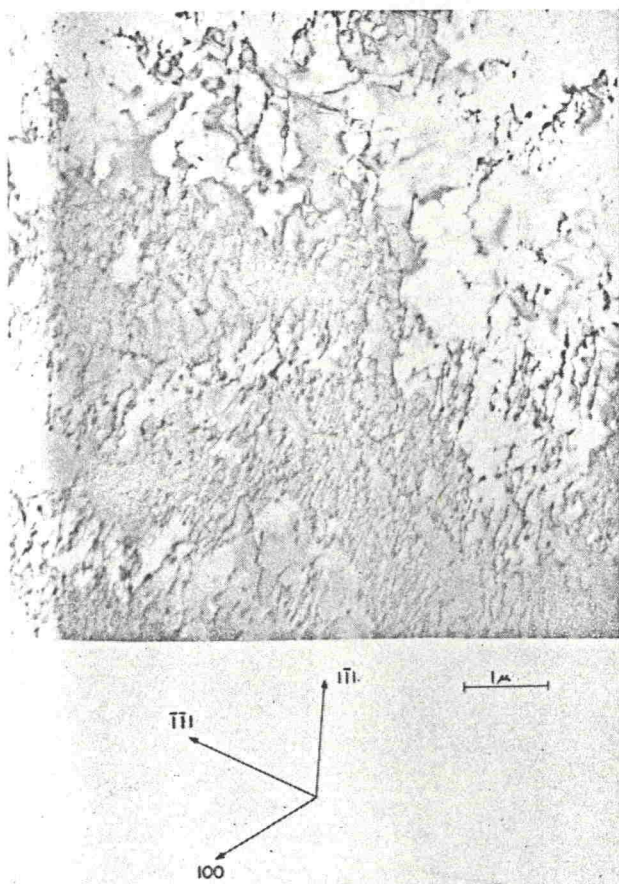


Fig. 13. Stage III, $\epsilon = 0.76$, section parallel to (011), $g = (2\bar{1}1)$. This type of network structure which is similar to that observed at $\epsilon = 0.63$ occurred over about half of the foil area.

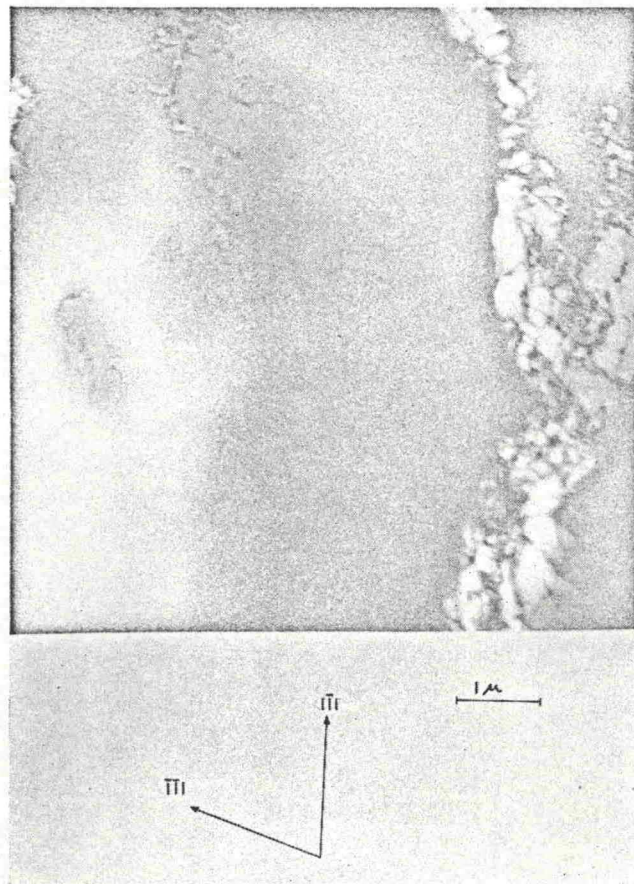


Fig. 14. Stage III, $\epsilon = 0.76$, section parallel to (011), $g = (2\bar{1}1)$. An elongated cell structure was observed over about half of the foil area. This is the first appearance of a cell structure in the primary slip plane and probably results from long range secondary slip occurring at this high strain.

boundaries of their own with misorientations that will be apparent in the (011) plane. The tangles still seem to line up along $\langle 111 \rangle$ directions. The appearance of these two different types of structure in these foils suggests that long-range secondary slip occurs giving rise to the cell appearance, whereas, the network structure is present in regions where long-range secondary slip has not penetrated.

3.5 Dislocation density measurements

Dislocation densities have been measured by counting intersections with random lines drawn on at least four enlarged micrographs for each strain.⁽¹⁵⁾ These were representative of the dislocation distributions observed in the specimens. The dislocation density of the as-grown crystals was estimated by counting the number of dislocations in a given area and was found to be about 10^7 cm^{-2} . Figure 15 is a plot of the square root of the dislocation density versus the shear stress. The straight line through the points satisfies the following relation:

$$\tau = 0.3GbN^{\frac{1}{2}} \quad (1)$$

where N is the dislocation density. The proportion of dislocations with each of the $(a/2)\langle 111 \rangle$ Burgers vectors has not been measured thoroughly, but it is estimated that there are twice as many primary dislocations as secondary dislocations in stage I, while in stage II the densities of the primary and secondary dislocations are about the same.

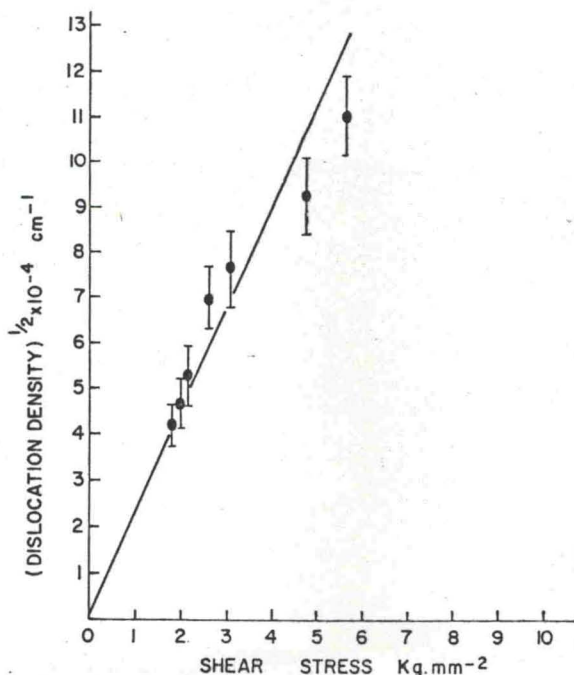


Fig. 15. Square root of dislocation density versus flow stress as determined from electron micrographs.

Since long-range secondary slip could not be detected either by X-ray methods or by changes of shape of the deformed single crystals,⁽²⁾ it is likely that the high secondary dislocation density originates from profuse short-range secondary slip, such as would occur to relieve the internal stresses developed around groups of primary dislocations. This has important consequences to work-hardening, as described in the next section.

4. DISCUSSION

The occurrence of three-stage hardening in tantalum single crystals over a limited range of orientations, temperatures and strain-rates has been thoroughly discussed previously.^(1,2) We are concerned here with the impact of the observed change of dislocation structure on the work-hardening behavior of tantalum. The dislocation distributions described in Section 3 may be interpreted as follows. In stage I dislocations tend to group together in tangles parallel to the primary slip plane. The tangles are surrounded by relatively dislocation-free areas such that the mean free path between them (and hence the slip distance) is large and the work-hardening rate is low. The tangles seem to be associated with regions containing a high density of small dislocation loops. This leads to the idea that the loops (formed by some mechanism such as double cross-slip) are the first permanent obstacles in the crystal and serve as nuclei for tangle formation by impeding glide dislocations. The observed dislocations are predominantly of screw orientation, although they are highly jogged. Presumably the slip distance of edge dislocations must be much greater than that of screw dislocations, i.e. screws are much less mobile than edges. A considerable number of secondary dislocations are observed even in stage I. The transition from stage I to stage II appears to be associated with a thickening of the tangles normal to the primary slip plane and a tendency for the tangles to be joined together by secondary dislocations lying out of the primary slip plane. As stage II proceeds the tangles increase in density and join up to form walls of dislocations approximately parallel to the primary slip plane; the walls are small-angle boundaries with misorientations across them that increase throughout stage II. The observed misorientations are $\sim \frac{1}{2}^\circ$. The walls contain many secondary dislocations with a density about the same as the primary dislocation density. The fact that alternate walls contain dislocations of opposite sign suggests that the secondary slip distance is equal to the separation of adjacent walls, which is thus much less than the primary slip distance due to the elongated nature of the cell structure. This structure continues

to develop into stage III with an increasing dislocation density and decreasing cell size. There is a tendency for the cell structure to become more equiaxed in stage III but this is probably due to the onset of large-scale conjugate slip as the tensile axis reaches the [001]-[101] symmetry boundary. Even at the highest deformations the dislocations tend to be mainly of screw orientation, although they are highly jogged and involved in complex networks. Reactions between dislocations of different Burgers vectors are observed at all stages of deformation; presumably $a\langle 001 \rangle$ reaction products are formed, although this was not confirmed.

The inhomogeneous dislocation arrangement described above is remarkably similar to that observed in f.c.c. metals (e.g. copper). There are important differences, of course, apart from the obvious differences in slip planes, burgers vectors and dislocation reactions; for example deformed f.c.c. crystals⁽¹⁶⁾ contain many edge dislocations and elongated edge dipoles and loops, whereas tantalum contains mostly screw dislocations and approximately circular dislocation loops.* Nevertheless, in both structures the development of a cell structure in stage II from the isolated tangles in stage I proceeds along very similar lines. The high secondary dislocation density and the occurrence of dislocation walls with misorientations across them suggest that localized secondary slip is being activated by the high internal stresses at the ends of newly formed slip lines, turning the groups of primary dislocations into boundaries without long-range stresses. Such behavior is just that required for the stage II work-hardening theory of Hirsch to be applicable.⁽¹⁹⁾ This theory has been quantitatively developed only for f.c.c. metals; we shall now adapt it to b.c.c. metals.

The model is that primary dislocations from sources pile-up at obstacles and the internal stresses around the pile-ups activate nearby secondary sources, converting the pile-ups into complex dislocation tangles which in turn act as obstacles to further slip. Since new tangles tend to form near other tangles (obstacles), an inhomogeneous dislocation structure, and eventually a cell structure, is naturally developed. Following through the calculations on similar lines to that for f.c.c. metals,⁽¹⁹⁾ we obtain the following

* The formation of edge dipoles and elongated loops in b.c.c. metals appears to be temperature dependent. In molybdenum crystals dipoles and elongated loops are observed after deformation at 575°K but not at room temperature and below (where mostly screw dislocations occur).⁽¹⁷⁾ Similarly in niobium, dipoles and elongated loops are observed at room temperature but not at lower temperatures.⁽¹⁸⁾ In tantalum, dipoles and elongated loops may occur after deformation at temperatures above 373°K but this has not yet been tested.

equation for the work-hardening rate in stage II:

$$\theta_{11} = \frac{G}{6\pi} \left(\frac{R}{D} \right) \left(\frac{a_s}{a} \right) \quad (2)$$

where R is the effective radius of an obstacle, D is the average distance between obstacles, a_s is the distance normal to the pile-up over which the total stress (external plus internal) is high enough to activate secondary sources, and a is the length of a pile-up of dislocations. The criterion for evaluating (a_s/a) is that secondary sources operate in regions where the total stress on a secondary system (applied stress τ_a' plus internal stress τ_{int}') is greater than the flow stress on a secondary system:

$$\tau_a' + \tau_{int}' > p\tau_a \quad (3)$$

where τ_a is the flow stress (applied stress) on the primary system and p is an overshoot factor which allows for the fact that the flow stress on a secondary system can be greater than that on a primary system. According to measurements of overshoot in tantalum single crystals it was found that $p \sim 1.05$.⁽²⁾ This value for p is a measure of the hardening on the conjugate slip system but it will be assumed to be the same for all the other secondary systems. Therefore equation (3) becomes

$$\frac{\tau_{int}'}{\tau_a} > 1.05 - \frac{\tau_a'}{\tau_a} \quad (4)$$

The ratio τ_a'/τ_a is a purely geometrical factor which depends on the particular secondary system under consideration and the orientation of the tensile axis within the standard stereographic triangle. For f.c.c. crystals τ_{int}'/τ_a can be calculated by resolving the stress field around a pile-up onto the various $\{111\}$ $\langle 110 \rangle$ secondary systems.^(20,21) For b.c.c. crystals, it simplifies matters to assume that slip occurs on $\{110\}$ planes rather than maximum resolved shear stress planes; this should not make too much difference in the final answer. Using $\{110\}$ $\langle 111 \rangle$ slip systems, it is apparent that the stress fields on secondary systems calculated for f.c.c. crystals can be used directly for b.c.c. crystals, since the slip planes and directions are simply interchanged. The values of τ_{int}' for the various secondary systems in terms of the stresses around screw dislocation pile-ups lying parallel to the z -axis on the slip plane normal to the y -axis are given in Table 1. Assuming that only screw pile-ups are important is again a simplification which should not effect the final result too much. The values of τ_{int}' in Table 1 have been mapped out previously in units of τ_a .^(20,21) The ratio (a_s/a) can be evaluated from these mapped out stress fields by measuring the region normal to the pile-up where equation (4)

TABLE 1. Values of τ'_{int} on each of the secondary slip systems in terms of the stresses around screw pile-ups on the primary system

Slip system	τ'_{int}	Stress-field source
(011) [111] 4B*	τ_{yz}	(20)-Fig. 1
(101) [111] 1C	$\frac{1}{2} \tau_{yz}$	(20)-Fig. 1
(011) [111] 3C	$\frac{2}{3} \tau_{yz} + \frac{\sqrt{2}}{3} \tau_{xz}$	(21)-Fig. 1
(110) [111] 5C	$-\frac{1}{6} \tau_{yz} - \frac{\sqrt{2}}{3} \tau_{xz}$	(20)-Fig. 7
(011) [111] 3A	$\frac{2}{3} \tau_{yz} + \frac{\sqrt{2}}{3} \tau_{xz}$	(21)-Fig. 1
(101) [111] 2A	$\frac{1}{6} \tau_{yz} + \frac{\sqrt{2}}{3} \tau_{xz}$	(20)-Fig. 7
(110) [111] 6A	$\frac{1}{2} \tau_{yz}$	(20)-Fig. 1
(011) [111] 4D	$\frac{1}{3} \tau_{yz} + \frac{2\sqrt{2}}{3} \tau_{xz}$	(20)-Fig. 7
(101) [111] 1D	$\frac{1}{6} \tau_{yz} + \frac{\sqrt{2}}{3} \tau_{xz}$	(20)-Fig. 7
(110) [111] 6D	$-\frac{1}{6} \tau_{yz} - \frac{\sqrt{2}}{3} \tau_{xz}$	(20)-Fig. 7

* System notation is an adaptation of that used in the f.c.c. system (see for example Mitchell⁽²⁰⁾).

is satisfied. Values of (a_s/a) derived in this manner for the various secondary systems are given in Table 2. The values for τ'_a/τ_a are also given in Table 2 and were calculated for an orientation near [517] where stage II usually begins for the orientation of the specimen used.

To evaluate θ_{11} [equation (2)] it is necessary to take a suitable average value for (a_s/a) . An average is taken so that the influence of all the secondary systems on the work-hardening behavior in stage II can be taken into account. The method used for finding an average value for (a_s/a) was to consider the various reactions which could occur between a primary dislocation with Burgers' vector $(a/2)[111]$ and each of the secondary dislocations with Burgers' vectors $(a/2)[111]$, $(a/2)[\bar{1}\bar{1}1]$ and $(a/2)[1\bar{1}1]$. The reactions are of the type

$$\frac{a}{2} [1\bar{1}1] + \frac{a}{2} [\bar{1}11] = a [001]. \quad (5)$$

However, the product dislocation with Burgers' vector $a[001]$ may be glissile or sessile depending on the slip planes of the reacting dislocations. There are four types of reactions to consider, as follows:

(A) The product is sessile. This will happen if the original slip planes are at right angles.

(B) The product is completely glissile. This will happen if the reacting dislocations are both on the same slip plane.

(C) The product is glissile in one of the original slip planes.

(D) The product is only glissile in a slip plane which is different from both of the original slip planes. All of the reactions between the primary dislocations and the secondary dislocations are given in Table 2 and are classified by type according to the previous designations.

Reactions (A) and (D) appear to offer the best possibilities for a resistance to primary dislocation motion and the formation of stable networks in the

TABLE 2. Values of τ'_a/τ_a and a_s/a and reactions with dislocations of the primary system (011) [111] for each of the secondary systems of the b.c.c. lattice

Secondary slip system	Reaction product	Direction	Glide plane	Type of reaction	$\frac{\tau'_a}{\tau_a}$	$\frac{a_s}{a}$
(101) [111]	$a[001]$	[111]	(110)	D	0.41	0.29
(011) [111]	$a[001]$	[100]	sessile	A	0.21	0.38
(110) [111]	$a[001]$	[111]	(110)	C	0.21	0.19
(011) [111]	$a[010]$	[100]	sessile	A	0.89	1.00
(101) [111]	$a[010]$	[111]	(101)	C	0.30	0.24
(110) [111]	$a[010]$	[111]	(101)	D	0.59	0.44
(011) [111]	$a[100]$	in (011)	(011)	B	0.10	0.43
(101) [111]	$a[100]$	[111]	(011)	C	0.14	0.17
(110) [111]	$a[100]$	[111]	(011)	C	0.05	0.14

tangles. These reactions would produce resultant dislocations that would not be as glissile as the reacting dislocations; type (A) more so than type (D). Therefore, the criterion used for calculating an average value of (a_s/a) was to average over the four systems in Table 2 corresponding to the (A) and (D) type reactions. Using this criterion the value obtained was $(a_s/a) \sim 0.5$. Values for (a_s/a) were also calculated for various positions along the path of migration of the tensile axis from its initial position (Fig. 1) to the [001]-[101] boundary. The average values obtained were very similar to that obtained for the tensile axis at the [517] pole.

Using $(a_s/a) = 0.5$ equation (2) becomes

$$\theta_{11} = \frac{G}{12\pi} \left(\frac{R}{D} \right). \quad (6)$$

It remains to estimate (R/D) . For f.c.c. crystals, Hirsch⁽¹⁹⁾ estimates that $(R/D) \simeq \frac{1}{4}$, since on the average secondary dislocations come from a distance $\sim \frac{1}{2}D$ and this will be equal to the effective diameter of the obstacle $2R$. However, for b.c.c. metals it is very likely that (R/D) will be considerably less than $\frac{1}{4}$ because of the ease of cross-slip. The ease of cross-slip means that dislocations will be able to circumvent obstacles in some situations, thus reducing the effective value of R , and also that the pile-ups formed may not be so "perfect" as assumed in the calculations, i.e. the dislocations may not all lie on exactly the same plane so that the resultant stress-field may be less than for a perfect pile-up.

In order to obtain the experimentally observed result (1-3.5)

$$\theta_{11} \simeq \frac{G}{600} \quad (7)$$

for b.c.c. metals it is necessary to reduce R by a factor of 4 as compared to the f.c.c. system, i.e. $(R/D) \sim \frac{1}{16}$ in b.c.c. crystals. All that can be said at this time is that this value does not appear unreasonable.

The relation between flow stress, τ , and dislocation density, N , based on Hirsch's theory⁽¹⁹⁾ is given by

$$\frac{\tau}{GbN^{\frac{1}{2}}} = \frac{n^{\frac{1}{2}}}{2\pi} \left(\frac{a_s}{a} \right) \quad (8)$$

where n is the number of dislocations in a pile-up.

From equation (1) and using the average value for $(a_s/a) \sim 0.5$, the number of dislocations in a pile-up in tantalum turns out to be $n \sim 14$. However, there is no experimental data to verify this value.

Of course, some of the factors in these calculations are very uncertain and more detailed calculations are required. Nevertheless, in view of the fact that the model follows the experimental observations very closely, the theory is likely to be appropriate to the stage II hardening region of b.c.c. metals. Indeed the theory should be applicable to a wider range of materials, especially those showing three-stage hardening.

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