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ON THE MICROMECHANISMS OF ANOMALOUS SLIP IN BCC METALS

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Abstract - Dislocation substructures developed in high-purity Mo single crystals deformed under uniaxial compression at room temperature to a total strain of ~0.5 % with a strain rate of 1 s^{-1} have been investigated using transmission electron microscopy (TEM) techniques in order to elucidate the underlying micromechanisms of the anomalous operation of $\{0\bar{1}1\}$ slip systems, i.e. Schmid-law violation, in bcc metals. The crystals were oriented with the stress axis parallel to a nominal single-slip orientation of $[\bar{2}\ 9\ 20]$, in which the $(\bar{1}01)$ [111] slip system is the only system having a maximum value of Schmid factor (m = 0.5). Nevertheless, the recorded stress-strain curve reveals no singe-slip or easy-glide stage, and the anomalous slip occurs in both (011) and $(0\bar{1}1)$ planes. TEM examination of the dislocation structure in the $(\bar{1}01)$ primary slip plane reveals that in addition to the operation of the $(\bar{1}01)$ [111] slip system, the coplanar $(\bar{1}01)$ $[1\bar{1}1]$ slip system that has a much smaller Schmid factor (m = 0.167) is also operative. Similarly, the $(0\bar{1}1)$ [111] slip system (m = 0.25) is cooperative with the coplanar $(0\bar{1}1)$ $[\bar{1}11]$ system (m = 0.287), and the (011) $[1\bar{1}1]$ slip system (m = 0.222) is cooperative with the coplanar (011) $[11\bar{1}]$ system (m = 0.32). The occurrence of $\{0\bar{1}1\}$ anomalous slip is accordingly proposed to be initiated from the cooperative dislocation multiplication and mutual trapping and blocking of 1/2[111] and 1/2$[1\bar{1}1]$ coplanar dislocation arrays in the $(\bar{1}01)$ plane. The resulted internal stresses render the propagation of both 1/2[111] and 1/2$[1\bar{1}1]$ screw dislocations from the $(\bar{1}01)$ plane onto the $\{0\bar{1}1\}$ planes and subsequently result in the occurrence of anomalous slip.

Introduction

Computer simulation and empirical studies of dislocation core structures in bcc metals for the last few decades have contributed greatly in interpretation of many peculiar mechanical behaviors of bcc metals such as tension/compression stress asymmetry, high Peierls (friction) stress for the propagation of screw dislocations, and strong strain-rate and temperature dependence of the yield and flow stresses [1], yet the core structure model alone remains insufficient to elucidate a certain peculiar behaviors of bcc metals such as anomalous slip that is occurring on planes for which the Schmid factors are fifth and sixth in the order of largest Schmid factors for {110}<111> slip systems, and for which the resolved shear stress is less than half that on the primary system. Although numerous and intensive studies have been made for the last four decades since Duesbery [2] first reported the occurrence of anomalous slip in Nb single crystals in 1969, its governing mechanisms remain controversial and mysterious [3-9]. Numerous reports have indicated that anomalous slip in general accompanies by a high work-hardening rate with planar, fine, and diffuse slip traces, which is in contract to a low work-hardening rate with coarse and wavy slip traces when anomalous slip becomes absence. Progress has recently been made to rationalize the anomalous slip phenomenon from a preliminary study of dislocation structure in Mo crystals (which were nominally oriented for single-slip) compressed at room temperature to a total-strain of 0.5% with a strain rate of 1 s^{-1}. The objective of this study is therefore aimed to characterize the evolution and transformation of dislocation structures in ultrahigh-purity Mo single crystals in order to elucidate the underlying micromechanisms that govern work hardening and anomalous slip (i.e. Schmid-law violation) in bcc metals.

Experimental

Mo single crystals were obtained from Accumet Materials Company, NY, which were grown by a two pass zone-refinement. The as-received sample then was decarburized at 1800 °C for 460 hours under an oxygen partial pressure of 2.1×10^{-6} Torr, followed by a 24-hour bake at 2300 °C under ultrahigh vacuum (UHV) conditions (10^{-11} Torr). The residual resistively ratio was raised from 1890 for as-received sample to 4458 for UHV purified sample. Prior to compression test, the test sample was heat treated at 1500 °C for 1 h, 1200 °C for 1 h, and 1000 °C for 1 h at a vacuum of 8×10^{-11} Torr. Testing of single crystals involves compressing the test sample between two platen surfaces under precise conditions. To measure shear strain during compression, a 3-element rosette gauge was bonded in the gauge section on each side of the sample. The gauges were applied with room temperature curing epoxy adhesive. A compression test was performed on a single-crystal sample oriented with a stress axis parallel to a nominal singe-slip orientation of $[\bar{2}\ 9\ 20]$, in which the primary slip system of $(\bar{1}01)\ [111]$ is the only one among the twelve slip systems having a maximum value of Schmid factor as shown in Table 1. The crystal was then compressed at a nominal strain rate of 1 s^{-1} to approximately 0.5 % axial strain. TEM foils were sliced from the gauge section of the tested piece with the foil sliced parallel to the $(\bar{1}01)$, $(0\bar{1}1)$, and (011) planes. TEM specimens were finally prepared by a standard twin-jet electropolishing technique in a solution of 75 vol.% ethanol and 25 vol.% sulfuric acid at ~25 V and -10 °C.

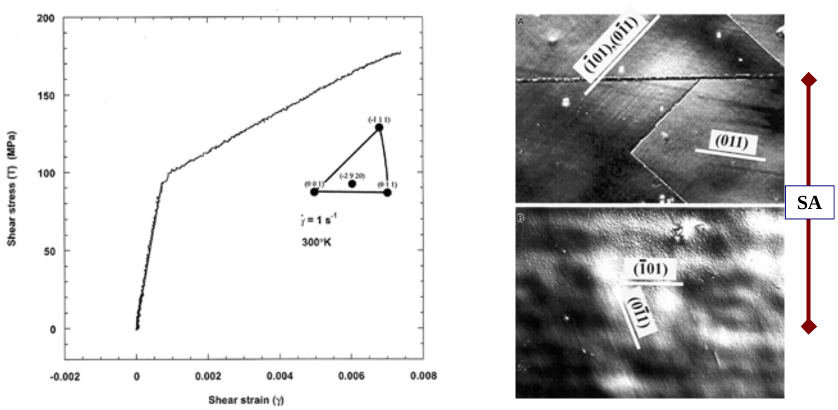
Sequence	Slip System	Schmid Factor (m)
1	$(\bar{1}01)\ [111]$	0.5
2	$(101)\ [\bar{1}11]$	0.47
3	$(011)\ [\bar{1}\bar{1}1]$	0.32
4	$(0\bar{1}1)\ [\bar{1}11]$	0.287
5	$(0\bar{1}1)\ [111]$	0.25
5	$(\bar{1}10)\ [111]$	0.25
7	$(011)\ [1\bar{1}1]$	0.222
8	$(101)\ [\bar{1}\bar{1}1]$	0.197
9	$(110)\ [\bar{1}11]$	0.183
10	$(\bar{1}01)\ [1\bar{1}1]$	0.167
11	$(\bar{1}10)\ [\bar{1}\bar{1}1]$	0.12
12	$(110)\ [1\bar{1}1]$	0.053

Table 1. Schmid factors of {011}<111> slip systems in the $[\bar{2}\ 9\ 20]$-oriented Mo crystal.

Result and Discussion

Stress-strain curve and slip trace analysis

The stress-strain curve recorded from the uniaxial compression of a $[\bar{2}\ 9\ 20]$–oriented Mo crystal and the optical metallography taken from two surfaces of the tested crystal are shown in Figures 1a and 1b, respectively. It can be readily seen that work-hardening occurred immediately after yielding, and no single-slip or easy-glide stage was recorded. In addition, the optical metallography reveals the formation of fine and diffused multiple slip traces in accompany with relative coarse and localized $(0\bar{1}1)$ and (011) slip traces.

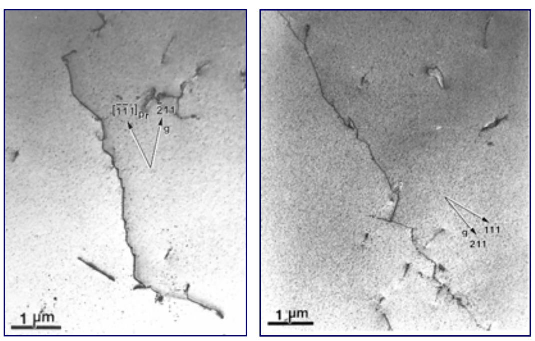


(a) (b)

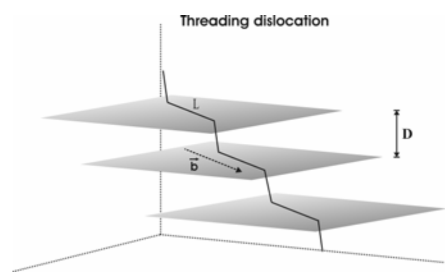
Fig. 1. (a) The stress-strain curve recorded from the uniaxial compression of a $[\bar{2}\ 9\ 20]$–oriented Mo crystal; (b) The optical metallography taken from two surfaces of the tested crystal showing the anomalous slip.

Dynamic dislocation multiplication

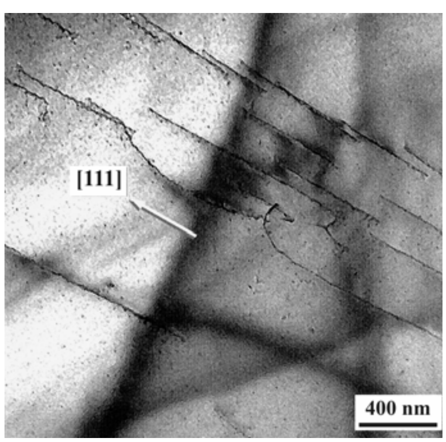
The initial dislocation structures in purified and annealed Mo crystals are found to contain numerous isolated and bended dislocation lines (with a dislocation density in the range of $10^6 \sim 10^7$ cm^{-2}) on which numerous kink and jog segments were observed as shown in Figure 2a. These segmental features of dislocation line actually make the 1-D line defect physically occupying a 3-D space in a crystal as illustrated in Figure 2b. That is, each dislocation line can be considered as a long threading dislocation with numerous segment portions resting on various slip planes within the crystal. Since jog segments can act as effective pinning obstacles for the motion of screw dislocation line, it is accordingly postulated that each segment portion of a threading dislocation can multiply and interact one another very differently under different loading conditions. It is suggested that the jogged screw dislocations can act as a dynamic multiplication source for dislocation multiplication when deformed at quasi-static conditions as a result of stress-induced migration and coalescence of super-jogs. The jog coalescence can take place via the lateral migration (drift) of jog segments driven by unbalanced partials of line tension acting on line segments (between jogs) of unequal lengths as shown and illustrated in Figures 2c and 2d. The coalescence of jog segments leads to the increase of both segment length and jog height. The jog coalescence continues until the segment length and jog height are greater than critical values so that applied stress begins to push each line segment to precede multiple dislocation multiplication. It is interesting to note from [10] that since jog segments can act as effective pinning obstacles for the motion of screw dislocation line, and the multiplication and interaction between segment lines will be very sensitive to the loading conditions. While very few dislocation dipoles (debris) were formed within sample compressed under a strain-rate of 10^{-3} s^{-1} (Figure 2e), a significant increase of dipoles (debris) were formed within sample compressed under a strain-rate of 1 s^{-1} (Figure 2f).



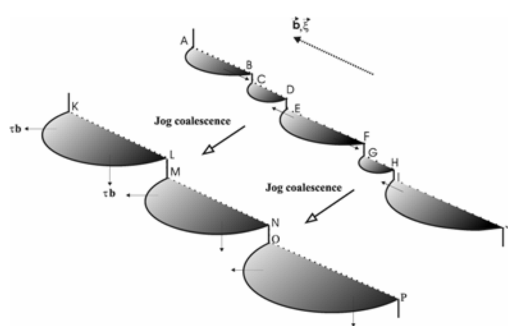
(a)



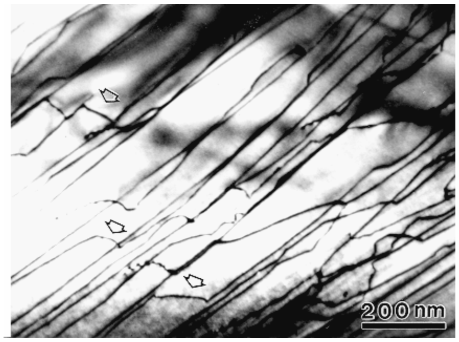
(b)



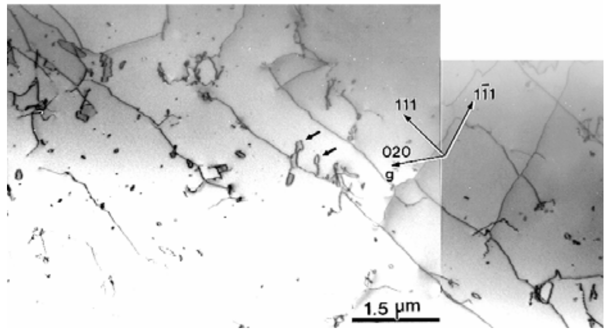
(c)



(d)



(e)



(f)

Fig. 2. (a) A typical TEM image showing numerous kink- and jog-segments formed along the initial dislocation lines of an annealed Mo crystal; (b) A schematic illustration of a jogged 1-D line defect that is physically occupying a 3-D space; (c) A typical TEM image showing the bowing of several screw dislocation segments within a deformed sample; (d) a schematic illustration of the development of multiple dislocation sources evolving from a jogged dislocation line through a jog coalescence process resulting from the unbalanced line-tension caused by the unequal-length of free segments; (e) A TEM image showing ½[111] screw dislocations associated with super-jogs (indicated by arrows) within a sample deformed under a strain rate of 10^{-3} s^{-1} [10]. (f) A TEM image showing the formation of numerous dislocation dipoles (debris) within a sample deformed under a strain-rate of 1 s^{-1}, and notice that two dipoles (marked by arrows) were pinched off from a screw dislocation line [10].

Cooperative dislocation multiplication and micromechanisms of anomalous slip

The deformation substructures observed within foils sliced parallel to the $(\bar{1}01)$, $(0\bar{1}1)$, and (011) slip planes revealed the formation of coplanar screw-dislocation arrays such that the 1/2[111] (m = 0.5) and $1/2[1\bar{1}1]$ (m = 0.167) coplanar arrays in the $(\bar{1}01)$ primary slip plane, the 1/2[111] (m = 0.25) and $1/2[\bar{1}11]$ (m = 0.287) coplanar arrays in the $(0\bar{1}1)$ plane, and $1/2[1\bar{1}1]$ (m = 0.222) and $1/2[11\bar{1}]$ (m = 0.32) coplanar arrays in the (011) plane. A typical example of coplanar dislocation arrays in $(\bar{1}01)$ is shown in Figure 3. More interestingly, the pile-up of screw dislocation arrays resulting from the mutual trapping of the coplanar arrays were frequently observed in these three slip planes. A typical observation of the mutual trapping and pile-up of screw dislocations in $(\bar{1}01)$ is shown in Figures 4a and 4b. These observations reveal that different from the mutual interception or cutting of dislocation lines that generally takes place during multiple-slip deformation, the operation of coplanar dislocation arrays occurs mainly in planes that are parallel to each other. Mutual trapping and blocking of coplanar arrays become feasible when they glide in the same plane or in planes that are very close to each other. The mutual trapping of screw dislocation arrays also indicates that the cross-slip of screw dislocations in Mo is difficult at room temperature.

The cooperative operation of coplanar dislocation arrays leads a heavy traffic scenario and results in a high local stress concentration in Mo deformed at ambient and low temperatures. It is accordingly suggested that the initial screw dislocations associated with "grown-in" superjogs can act as effective sources for multiplying both 1/2[111] (Schmid factor = 0.5) and $1/2[1\bar{1}1]$ (m = 0.167) coplanar screw dislocation arrays in the $(\bar{1}01)$ primary slip plane. The (Peach-Kohler) interaction force between the freshly multiplied 1/2[111] screw dislocations and $1/2[1\bar{1}1]$ screw dislocations results in the multiplication of $1/2[1\bar{1}1]$ screw dislocations, which leads to the formation of 1/2[111] and $1/2[1\bar{1}1]$ cross-grid dislocation arrays in the $(\bar{1}01)$ primary slip plane. The occurrence of $\{0\bar{1}1\}$ anomalous slips is intimately related to the onset of a cascade event of dislocation multiplication and propagation caused by the internal stresses originating from the interactions between the cooperative screw dislocation arrays. The internal stresses render the propagation of 1/2[111] and 1/2$[1\bar{1}1]$ screw dislocations from the primary slip planes onto the $(0\bar{1}1)$ and (011) planes and subsequently resulting in the anomalous operation of slip systems in the $(0\bar{1}1)$ and (011) planes, in which the slip systems should be inoperative according to Schmid law. A typical example of the cross-slip of 1/2[111] dislocations at local region of a $(\bar{1}01)$ slip band onto $(0\bar{1}1)$ is shown in Figure 4c.

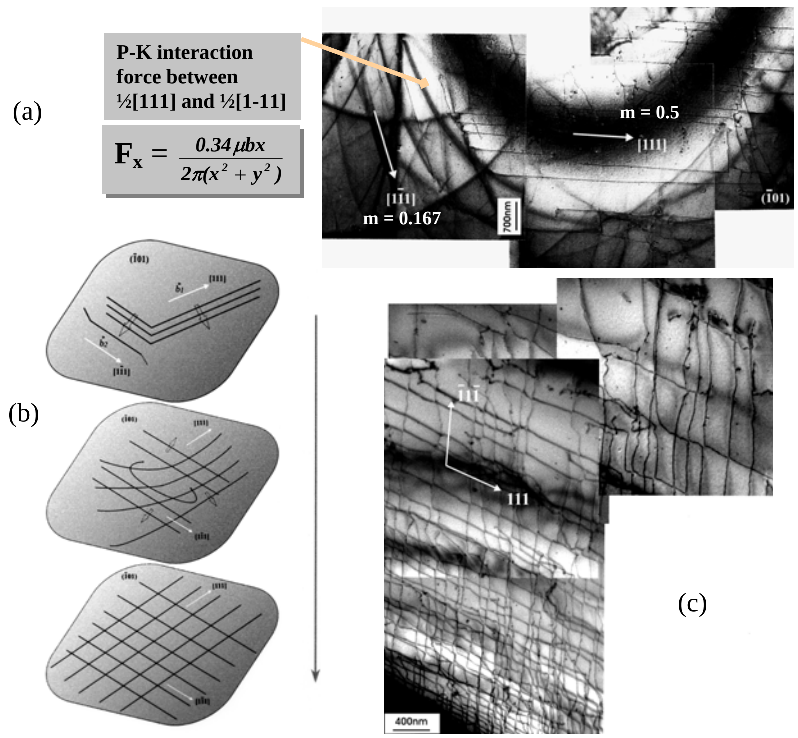
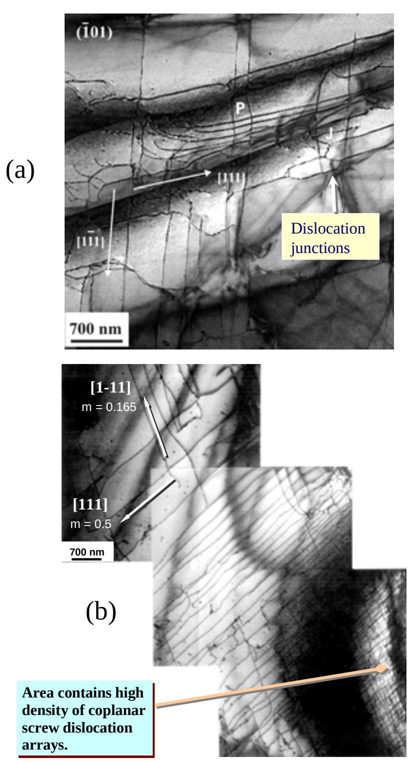


Fig. 3. (a) A TEM image showing the interaction between a newly formed ½[111] dislocation array and pre-existing ½$[1\bar{1}1]$ dislocation segment; (b) A schematic representation of the cooperative multiplication of a coplanar dislocation array; (3) A TEM image showing the formation of coplanar dislocation arrays in $(\bar{1}01)$.



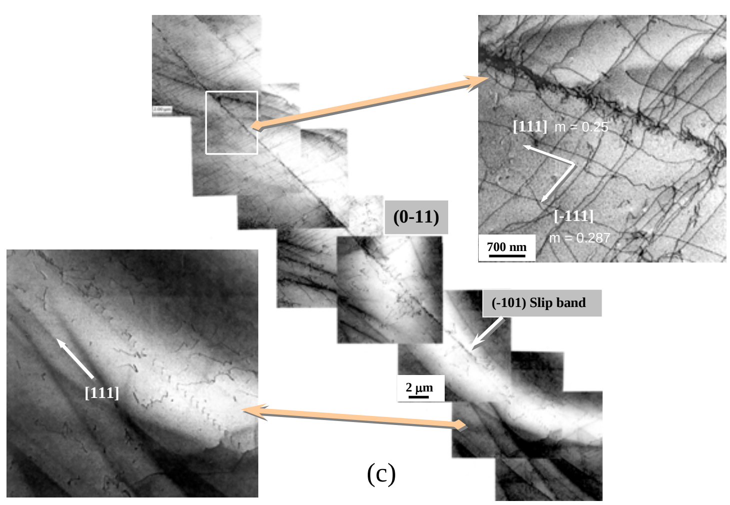


Fig. 4. (a) A typical observation of the pile-up of screw dislocation array in front of a dislocation junction in $(\bar{1}01)$; (b) The mutual trapping of coplanar dislocation arrays in $(\bar{1}01)$; (c) A typical observation of the cross-slip of 1/2[111] dislocations at local region of a $(\bar{1}01)$ slip band onto $(0\bar{1}1)$.

Since the occurrence of anomalous slips in Mo crystals is intimately related to the cross slip induced by the local stress concentration resulting from the mutual trapping of coplanar dislocation arrays, it is accordingly suggested that the anomalous slip phenomenon in bcc metals is governed by the easiness of dislocation cross-slip, which in turn depends strain rates and testing temperatures. That is, when cross-slip of screw dislocations becomes prevalent under high-temperature and low strain-rate conditions, the mutual trapping and pile-up of screw arrays becomes less likely, and thus the anomalous slip phenomenon will be suppressed. Since the cascade event of cooperative dislocation multiplication, mutual trapping, and propagation of dislocations will lead to a rapid increase of dislocation density within the single-slip oriented crystal, it is anticipated that work-hardening stage appears immediately after yielding.

Conclusion

The subject of anomalous slip phenomenon in bcc metals has been revisited by examining the dislocation substructures developed within Mo single crystals deformed under uniaxial compression at room temperature to a total strain of ~0.5 % with a strain rate of 1 s^{-1}. The results reveal that the initial screw dislocations associated with "grown-in" super-jogs can act as an effective source for multiplying both 1/2[111] (Schmid factor = 0.5) and $1/2[1\bar{1}1]$ (Schmid factor = 0.167) coplanar screw dislocation arrays in the $(\bar{1}01)$ primary slip plane. The interaction between the newly multiplied 1/2[111] dislocations and pre-existing $1/2[1\bar{1}1]$ dislocation segments renders the multiplication of $1/2[1\bar{1}1]$ dislocations, which in turn leads to the formation of both 1/2[111] and $1/2[1\bar{1}1]$ dislocation arrays in the $(\bar{1}01)$ primary slip plane. The occurrence of $\{0\bar{1}1\}$ anomalous slip is accordingly proposed to be initiated from the event of dislocation multiplication and propagation caused by the mutual trapping and blocking of 1/2[111] and $1/2[1\bar{1}1]$ coplanar dislocation arrays in the $(\bar{1}01)$ slip plane. The resulted internal stresses render the propagation of both 1/2[111] and $1/2[1\bar{1}1]$ screw dislocations from the $(\bar{1}01)$ plane onto the $\{0\bar{1}1\}$ planes by a cross-slip process, which subsequently results in the anomalous operation of slip systems in the $\{0\bar{1}1\}$ slip planes.

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