Orientation Dependence of the Temperature of Brittle-Ductile Transition of Molybdenum Single Crystals

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Abstract. The effect of single crystal orientation on the temperature of the brittle-ductile transition of molybdenum was studied. It is revealed that the mechanism of fracture depends on both temperature of deformation and orientation of single crystals. The mechanism of fracture by cleavage is gradually replaced by plastic fracture with increasing $\xi$ angle. The orientation dependence of the temperature of the brittle-ductile transition was established.

Introduction
The temperature of the brittle-ductile transition $T_{bd}$ in bcc metals is substantially influenced by grain size, pressure, rate of deformation, and texture of investigated material. Together with these factors one would expect that $T_{bd}$ should depend on the orientation of the single crystals. However, despite the importance of this issue for the understanding of the mechanism of fracture of bcc metals, there is practically no published information on the effect of orientation of single crystals on $T_{bd}$. This paper is devoted to establishing the character of dependence of $T_{bd}$ of molybdenum single crystals on their orientation.

Experimental
High-purity single crystals of molybdenum were used for the investigation. The resistivity ratio $R_{300K}/R_{4.2K}$ was 2,000. The specimens were in the shape of parallelepips 2.0x0.2 mm\(^2\) in cross-section and 16 mm long. The orientations of the longitudinal axes of the single crystals were selected along the boundary $[00\overline{T}] \sim [\overline{1} \overline{T} \overline{T}] \sim [\overline{1} \overline{T} 0]$ of the main stereographic triangle (Fig. 1). The $\xi$ angle, characterizing orientation of single crystal, is the angle between the plane $(00\overline{T})$ and the plane having maximal normal stresses [1]. The orientations of the single crystals were determined by the X-ray Laue black-reflection method with $2^\circ$ precession. Specimens having various orientations were strained by tension to fracture at temperatures of 77, 173, 223, 293, 333, 373, 413, 473 and 523 K. The tension rate was fixed and equal to $2\times10^{-6}$ m/s.

Results and Discussion
The study of the deformation of molybdenum single crystals has revealed that if the deformation temperature is above 413 K, the single crystals of all the investigated orientations are fractured only by plastic rupture with formation of blade-type ends (Fig. 2). At 77 K, the fracture of single crystals of all orientations occurs only by brittle cleavage along planes belonging to the family of $<111>$ zone. However, in the range of intermediate deformation temperatures lying within 173 to 373 K, the character of the fracture of the molybdenum single crystals depends considerably on their orientation. At each temperature, as the $\xi$ angle increases, brittle fracture by cleavage is gradually replaced by plastic rupture. In general, this trend is the same for all deformation temperatures in the
range of 173–373 K. However, with decreasing deformation temperatures, the boundary separating the region of orientations of single crystals featuring brittle fracture from the one with plastic fracture is continuously displaced in the direction of greater $\xi$ angles. Such a displacement of the boundary continues until at 77 K molybdenum single crystals become fully brittle for all $\xi$ angles.

![Diagram](image_url)

**Fig. 1.** Orientations of the longitudinal axes of molybdenum single crystals.

We take the deformation temperature at which a neck begins to form on the surface of specimens as the temperature of brittle-ductile transition $T_{bd}$. The values of $T_{bd}$ thus obtained for molybdenum single crystals are shown in Fig. 3 as a function of their orientation (dotted line). It is evident that with an increase of the $\xi$ angle, $T_{bd}$ gets displaced into the region of lower temperatures, the total drop of $T_{bd}$ attaining ~200°, with angle $\xi$ varying from 0 to 90°. The continuous line limits region in which ductile fracture is carried out by formation of blade-type ends (region 1). In the region between continuous and dotted lines final fracture occurs by brittle cleavage.

The existence of an orientation dependence of $T_{bd}$ in molybdenum single crystals is the main reason for the anisotropy of their plastic properties [2,3] in the case of deformation at a constant temperature. It follows from the obtained results that the anisotropy of plastic properties will be observed only in the event that the deformation of molybdenum single crystals occurs in the temperature range of 173–373 K.

The border dividing the region of orientations of single crystals with brittle fracture from the region of orientations of single crystals with ductile fracture for different temperatures deformation is shown in the basic stereographic triangle (Fig. 4). When temperature of deformation decreases the region of orientations of single crystals with brittle fracture is formed primary near pole $<001>$. At the further decrease of temperature this region increases in size and is displaced to pole $<011>$ and at 77 K single crystals of all of orientations will be ruptured only brittle. Thus the border of change of the mechanism of fracture is not constant and it is a function of temperature of deformation.

In accordance with accepted concepts, the change in the fracture mechanism with a decrease of temperature is due to the different temperature behaviour of the yield strength $\sigma_y$ and the brittle fracture stress $\sigma_f$. In our case, as the single crystal orientation changes, the change in the fracture mechanism occurs at a constant deformation temperature. The cause of the change of mechanism is the same from the physical point of view: with an increase of the $\xi$ angle, the critical fracture strength does not remain constant, but increases. This follows from the results in [1], wherein it is shown that with a change of single crystal orientation there occurs a replacement of the active cleavage plane, and, hence, a change in the critical fracture stress. As a result, as the $\xi$ angle varies...
Fig. 2. Summary picture of photos of the surface of fracture of molybdenum single crystals with different values $\xi$ deformed at various temperatures. Pointers show position of blade-type ends.
Fig. 2 (continuation). Summary picture of photos of the surface of fracture of molybdenum single crystals with different values $\xi$ deformed at various temperatures. Pointers show position of blade-type ends.

- 293 K
- 223 K
- 173 K
- 77 K

$\xi = 49^\circ$ $\xi = 63.5^\circ$ $\xi = 76^\circ$
Fig. 3. Orientation dependence of the temperature of brittle-ductile transition of molybdenum single crystals:
1 – the region of ductile fracture, 2 – the region of brittle fracture;
$T_1$ – temperature of the beginning of ductile fracture for $\xi = 0^\circ$; $T_2 = 77$ K;
$T_3$ – temperature of brittle-ductile transition for $\xi = 0^\circ$.

Fig. 4. Orientations of molybdenum single crystals with brittle and ductile fracture at various temperatures of deformation:
○ – fracture occurs brittle; ● – fracture occurs ductile.
from 0 to 90° the critical fracture stress increases $\sigma_f$ by a factor of almost 2.5 (Fig. 5). The yield stress does not remain fixed, but varies also as the single crystal orientation is altered. However, this change is much less than the variation of the critical fracture stress. That is why $\sigma_s$ changes somewhat with variation of the $\xi$ angle, while $\sigma_f$ grows. The change in the fracture mechanism occurs only for those $\xi$ orientations, for which $\sigma_f$ becomes equal to $\sigma_s$. Single crystals with $\xi < \xi_o^{T}$ have a yield strength higher than the critical fracture stress for the corresponding crystallographic plane. In this range of orientations we observe only brittle fracture of the single crystals. For orientations $\xi > \xi_o^{T}$ the yield strength is found to be substantially less than the fracture stress, and single crystals having such orientations experience plastic deformation until full separation occurs. Thus, angle $\xi_o^{T}$ characterizes such an orientation of molybdenum single crystals for which there exists an equality between the yield stress and fracture stress. From the physical point of view, this value of angle $\xi_o^{T}$ has a corresponding temperature $T_{bd}$ in the event the fracture mechanism changes as the deformation temperature varies. With a change of single crystal orientation, the equilibrium between the yield strength and fracture stress disappears. As a result, the material passes either into the plastic or brittle state depending on the $\xi$ angle.

Fig. 5. The scheme explaining transition from brittle fracture to ductile fracture:
$\sigma_f$ – fracture stress; $\sigma_s^{T}$ – yield strength at deformation temperature $T$; $\sigma_s^{T_1}$ – yield strength at deformation temperature $T_1$; $T_1$ < $T$.

The variation of $\sigma_f$ and $\sigma_s$ with orientation makes it possible to explain the physical nature of the change in the fracture mechanism in the course of deformation at constant temperature. The special feature of the plastic deformation of bcc metals is the marked temperature dependence of the yield strength [4]. On the other hand, according to experimental data the brittle strength of metals exhibits a relatively weak dependence on temperature. Taking into account these two factors one can explain fully the temperature behaviour of $T_{bd}$. If the deformation temperature is lowered, the value $\sigma_f$ does not change, practically. On the contrary, because of the strong temperature dependence the yield strength $\sigma_s$ increases greatly with decreasing deformation temperature. As result, with a drop in deformation temperature the point $\xi_o^{T}$ is systematically displaced into the region of greater $\xi$ angle until the molybdenum single crystals become brittle at all orientations of the tension axis. Since the considered special features of the plastic deformation process are common to all bcc metals, one can assert that all bcc metals have an orientation dependence of $T_{bd}$ similar to that of molybdenum.
The only difference will be that this curve will lie in differing temperature intervals depending on the type of metal.

Conclusions

1. The orientation dependence of $T_{bd}$ of molybdenum single crystal has been established.
2. A physical explanation has been suggested for the anisotropy of plasticity and orientation dependence of $T_{bd}$ of bcc metals.

References