Cleavage Anisotropy in Tungsten Single Crystals

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We have performed an extensive study of the cleavage fracture of tungsten single crystals between 77 K and room temperature. The dependence of the fracture toughness on temperature and on crack propagation direction as well as the river line patterns on the fracture surfaces clearly indicate that the intrinsic brittle fracture process is anisotropic with respect not only to the plane but also to the direction of crack propagation. This anisotropy cannot be explained within Griffith's thermodynamic theory of brittle fracture. However, it compares well with atomistic simulations, which suggest that it may be a consequence of anisotropic lattice trapping. [S0031-9007(96)00159-7]

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A long-standing problem in brittle fracture is the prediction of the favorable cleavage planes in crystalline materials. Customarily, one resorts in this respect to the treatment of Griffith [1], which states that the energy released upon crack advance, the energy release rate G, must equal the surface energy γ of the two freshly exposed fracture surfaces: $G = 2\gamma$. Accordingly, only surfaces with the minimum surface energy should appear as favored cleavage planes [2]. However, a few clear exceptions to this rule are known, the most prominent being the {100} cleavage of the bcc transition metals. Despite the markedly lower surface energy of the close packed {110} surface [4,5], even the elastically (almost) isotropic metal tungsten primarily cleaves on {100} planes [6].

Attempts have been made to explain this discrepancy in terms of the plastic relaxation around differently oriented crack tips [7]. Despite some severe criticism of the method of analysis [8], the argumentation that the plastic relaxation around the crack tip is responsible for the selection of the cleavage plane in bcc transition metals has been widely accepted. However, this might also be due to a lack of alternative models.

Based on an atomistic study of brittle crack propagation in bcc transition metals, an alternative explanation has recently been put forward [9]. The atomistic simulation showed that the perfectly brittle cleavage process (on one individual cleavage plane) can be anisotropic with respect to the crack propagation direction within a given plane, leading to distinctly "easy" and "tough" crack systems (crack plane and propagation direction). According to this study, the {100} crack plane provides two crystallographically independent easy propagation directions orthogonal to each other. Therefore, an arbitrarily oriented crack front will always find a vehicle of one or two easy propagation directions. In contrast, on the {110} plane there is only one easy propagation direction, with a tough direction perpendicular to it. In consequence, an arbitrarily oriented crack front will seldom encounter favorable propagation directions. Therefore, {100} cleavage should generally be favored over {110} cleavage and the latter is expected to occur only for certain crack propagation directions.

Although the cleavage fracture of bcc transition metal single crystals, especially of tungsten, has already been studied several times [6,10,11], the available experimental data are still far too sparse to decide between the two approaches. Furthermore, only very limited knowledge has been acquired on {110} cracks and the influence of crack propagation direction has not yet been studied carefully.

We report on a series of fracture toughness tests on tungsten single crystals devised so as to differentiate between the two hypotheses concerning the preference of the {100} plane. We study the fracture toughness of the four low index crack systems [12] at different temperatures between room temperature and liquid nitrogen temperature (77 K). Decreasing the test temperature reduces dislocation mobility. One can, therefore, expect to be able to separate the contribution of plasticity and the intrinsic (brittle) fracture resistance of the crystal. Different macroscopic crack propagation directions within each of the crack planes are studied to test the predictions from atomistic modeling [9].

The toughness tests are performed on high purity W single crystal bars ($3 \times 6 \times 30$ mm^3) loaded in three point bending. The material [13] and details of the experimental techniques are described elsewhere [14]. All fracture specimens were precracked at 77 K using the composite bending technique [15], where the notched sample is loaded with a supporting steel bar until a (pre)crack pops in. The precrack length was first measured on the polished side surfaces and specimens were accepted for final testing only if the precracks had stopped between 0.45 and 0.7 of the total width of the specimen. The length of the precrack was evaluated from the compliance of the specimen and, where possible, also determined *post mortem* on the fracture surfaces. Both values usually agreed very well. Multiple tests (more than five) have been conducted for all four crack systems at room temperature and at 77 K and several individual tests at the temperatures in between. All

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toughness tests were performed with a constant loading rate which, due to variations in the length of the precrack, translate into almost constant stress intensity factor rates of 0.10 ± 0.02 MPa $\sqrt{\text{m}}$/s. The dependence of the measured fracture toughness on temperature is shown in Fig. 1 for all four crack systems.

The room temperature data as well as the 77 K results are also listed together with the predictions from atomistic calculations [9,16] in Table I. It is evident that both {110} crack systems have a significantly higher room temperature fracture toughness than the {100} crack systems. With decreasing temperature, however, the crack systems with ⟨110⟩ crack fronts, namely, the $\{100\}\langle 011\rangle$ and $\{110\}\langle 1\bar{1}0\rangle$ crack systems, are significantly easier to cleave than the crack systems with ⟨100⟩ crack fronts.

Most of the room temperature fracture specimens revealed small deviations from the linear elastic load displacement curves before final fracture, indicating a limited amount of plastic relaxation. The fracture surfaces are significantly rougher than those of the precracks and of the specimens tested at 77 K. Final cleavage was always catastrophic. Both types of {110} crack systems display {100} facets in the fracture surface.

Testing at 77 K always resulted in brittle cleavage fracture on the precrack plane for all four crack systems. The load-displacement curves showed perfectly linear elastic behavior up to the load at which fracture occurred. The fracture surfaces are clean except for a few river lines.

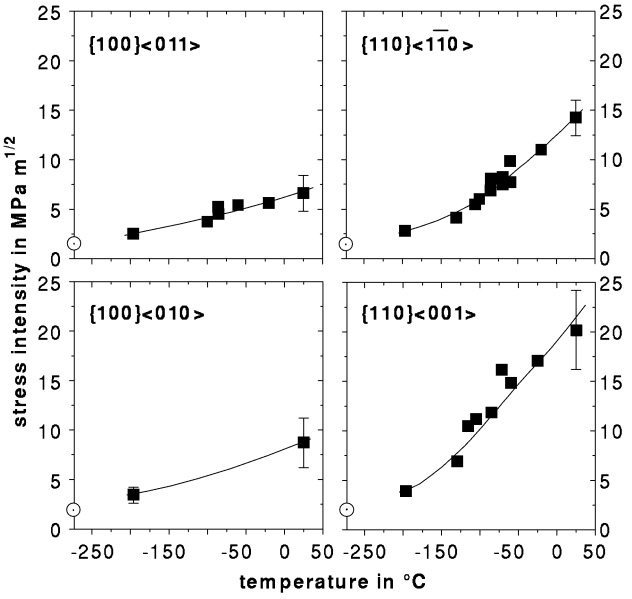

FIG. 1. Fracture toughness of tungsten single crystals for the {100} and {110} cleavage planes with crack front directions as indicated on the figure. At room temperature and at liquid nitrogen temperature (77 K) mean values and standard deviations from at least five measurements are indicated, whereas for the other temperatures individual measurements are given. The open circles are theoretical predictions from atomistic modeling.

TABLE I. Fracture toughness of tungsten single crystals for the {100} and {110} cleavage planes with different crack front directions. Data at room temperature (RT) and at liquid nitrogen temperature (77 K) are mean values and standard deviations from at least five individual measurements. Atomistic modeling results are almost identical to those of [9] but calculated with a somewhat improved loading procedure [16]. Fracture toughness is given in MPa m$^{1/2}$.

Crack system	RT exp.	77 K exp.	Atomistic modeling
$\{100\}\langle 010\rangle$	8.7 ± 2.5	3.4 ± 0.6	2.05
$\{100\}\langle 011\rangle$	6.2 ± 1.7	2.4 ± 0.4	1.63
$\{110\}\langle 001\rangle$	20.2 ± 5.5	3.8 ± 0.4	2.17
$\{110\}\langle 1\bar{1}0\rangle$	12.9 ± 2.1	2.8 ± 0.2	1.56

On the {100} crack surfaces river lines occur only at or near the location of the stopped precrack, whereas river lines are visible on the whole fracture surface of the {110} specimens. The river lines follow the macroscopic propagation direction for the two crack systems with ⟨011⟩ crack fronts. The river lines always deviate significantly from the macroscopic propagation direction in the $\{100\}\langle 010\rangle$ crack system (Fig. 2). They even tend to align themselves perpendicular to the macroscopic crack propagation direction in the $\{110\}\langle 001\rangle$ crack system. For the {100} cracks, similar observations have previously been reported from fracture experiments with small, spark induced precracks [6,11,18].

Both the qualitative observations and the measured fracture toughness values (Fig. 1) suggest that fracture at 77 K occurs in an almost perfectly brittle way for all four crack systems. The measured fracture toughness at 77 K is only about 50% higher than the calculated one (c.f. Table I), which may result from (1) a somewhat too low surface energy of the interatomic potential, (2) the slightly imperfect cleavage surfaces, and (3)

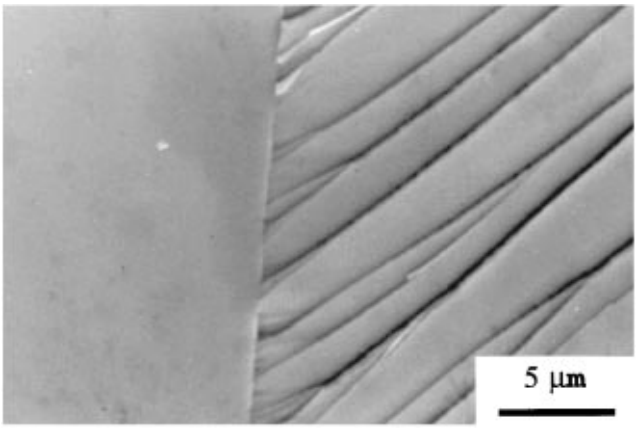

FIG. 2. {100} fracture surface with macroscopic crack front aligned along ⟨001⟩. Crack is propagating from the left to the right. Final fracture started from the central arrest line. River lines are aligned approximately along the ⟨011⟩ direction at 45° to the macroscopic propagation direction.

possible shielding of the crack by preexisting dislocations which are not fully immobilized at this temperature. Unfortunately, neither of these influences can be shown to be irrelevant but etching of the fracture surfaces [19] showed a few etch pits near the location of the stopped precrack. This suggests that the restarting of the crack in the final fracture experiment may still have been accompanied by some dislocation activity. Nevertheless, the differences in the measured 77 K fracture toughness between the cracks of different directions, within both cleavage planes, appear to be too large to be caused by these effects and one has to conclude that the perfectly brittle fracture process itself must be anisotropic with respect to crack propagation direction.

One arrives at the same conclusion if one compares the temperature dependence of the fracture toughness for the different cleavage systems (Fig. 1). While at room temperature both {110} crack systems show significant contributions from dislocation activity, the two {100} crack systems show much less of this. At 77 K, remaining dislocation activity should contribute less to the measured fracture toughness. However, since the fracture toughness of the $\{110\}\langle 0\bar{1}1\rangle$ crack system drops below both the other {110} crack system *and* the $\{100\}\langle 010\rangle$ crack system, one has to conclude that some other effects than dislocation activity must be important for the observed differences.

If the river lines are taken as a true indication of the local crack propagation direction, they yield further evidence for preferred crack propagation directions. The river line patterns suggest that crack propagation microscopically follows the $\langle 011\rangle$ directions on the {100} cleavage plane (c.f. Fig. 2) and the $\langle 001\rangle$ direction on the {110} cleavage plane. In both cases, these are the directions with the lowest resistance to propagation within each of the planes studied. The results therefore are internally consistent.

All qualitative observations and measurements therefore suggest that cleavage in tungsten is anisotropic with respect not only to the planes but also to the propagation direction. Since our results seem to rule out dislocation activity as the possible origin for this anisotropy and since tungsten even at 77 K is elastically almost isotropic, we conclude that the brittle fracture process itself must be anisotropic. Such an anisotropy to our knowledge can be interpreted only as an effect of the discrete atomistic nature of the crystal. On the atomic scale the breaking of the bonds will of course depend on the orientation of the bonds with respect to the main loading axis and the lattice trapping effect [21], which manifests itself in a finite stability range ΔK for a crack of given length, has indeed been shown to be anisotropic with respect to the orientation of the crack front on a given cleavage plane [9]. Although the lattice trapping effect is not sufficiently well understood to predict its magnitude and the dependence on loading conditions [22] *a priori*, its dependence on crack propagation direction is rather well established [9,22].

It remains to ask how an anisotropy in lattice trapping actually influences the measured fracture toughness. To shed some light on this question we may first interpret the trapped crack and its surround as a thermodynamic ensemble in the Griffith sense. The crack tip could then be interpreted as an entity moving on an oscillating energy surface. One would expect the crack to meander or jump forward and backward over the lattice trapping barrier but, in equilibrium, to remain at the length compatible with the Griffith energy balance. In this sense one can, for example, explain slow crack growth phenomena as a succession of equilibrium states [23]. For cleavage fracture, however, the picture is somewhat different. The crack is loaded steadily and driven up the energy surface (away from equilibrium) up to a point at which it can overcome the lattice trapping barrier and at which it will then start moving dynamically. Of course, the time scales and temperatures at which a crack can be treated thermodynamically as a succession of equilibrium states, and the time scales at which nonequilibrium thermodynamics comes into play and at which the crack is kinetically limited, strongly depend on the height of the lattice trapping barrier. However, it is important to note that in the dynamic regime, where we believe the low temperature cleavage fracture to be situated, fracture criteria derived from equilibrium theories like the Griffith criterion can only be regarded as necessary conditions but not as sufficient.

As far as the selection of crystallographically distinct cleavage planes is concerned, two models have been brought forward. In the first approach, the plastic relaxation around differently oriented crack tips is held responsible for the selection [7]. Specifically, for the bcc transition metals, {100} planes should be favored as cleavage planes over {110} planes because of the less favorably oriented glide systems. Qualitatively, this point of view would seem to be supported by our room temperature results. The temperature dependence of the fracture toughness, however, clearly shows that this argument cannot hold at 77 K. The level of fracture toughness is similar on both planes for cracks with a crack front along a $\langle 110\rangle$ direction. Therefore one could expect both planes to be similarly suitable as cleavage planes. However, there is an important difference between the two cleavage planes in the number and orientation of the easy propagation directions. In perfect agreement with the atomistic modeling [9] we find that cracks with $\langle 100\rangle$ crack fronts propagate less easily on both cleavage planes. Consequently, we regard the availability of four orthogonal easy propagation directions on the {100} crack plane as the major cause for its predominance as a cleavage plane. An arbitrarily oriented crack front will always find a vehicle of one or two easy propagation directions and will always exert a significant driving force along the easy directions. In contrast, an arbitrarily oriented crack front on the {110} plane will encounter only one easy propagation direction, and it will not be

able in general to follow it for more than a short distance until it is elongated along a crack front perpendicular to a tough propagation direction. From there on the crack will not move any further unless it is loaded high enough to overcome the higher lattice trapping barrier.

Finally it should be remarked that in the semibrittle regime a quantitative understanding of the increase of the fracture toughness with temperature is still lacking. Modeling of semibrittle fracture in bcc transition metals on the basis of dislocation velocity laws is currently in progress. Similarly experiments to determine the brittle to ductile transition temperature are under way and will be reported elsewhere.

In conclusion, we have performed fracture toughness tests on tungsten single crystals between 77 K and room temperature for the four low index crack systems. The quantitative results as well as the qualitative features of the fracture surfaces indicate that the cleavage process is anisotropic with respect to propagation direction within a specific cleavage plane. From the measured temperature dependence of the fracture toughness we can rule out plasticity as the origin of this anisotropy. We are forced to conclude that the anisotropy is a generic feature of the perfect brittle cleavage process. This conclusion is supported by previous atomistic simulations, which had indicated such a cleavage anisotropy; it was shown that the preference of {100} cleavage over {110} cleavage can be explained as a consequence of this anisotropy and the different number of easy directions on each plane. In general, such a cleavage anisotropy cannot be understood within conventional thermodynamic theory. It can, however, be explained as a consequence of anisotropic lattice trapping, which could provide a kinetic limitation to the fracture process. The results of this study therefore indicate that the (low temperature) brittle fracture process should be analyzed from an atomistic rather than a thermodynamic point of view.

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