MECHANISMS AND CRITERIA FOR CLEAVAGE

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ABSTRACT

Proposed criteria for predicting whether a material will behave in a 'brittle' or a 'ductile' manner are reviewed and modified to account for new experimental observations. Metallographic and fractographic studies of cleavage fracture have been made for iridium and zinc in inert environments and for an Al-Zn-Mg alloy, cadmium and α-titanium in liquid-metal environments. For the FCC metals (Ir, Al-Zn-Mg), cleavage fractures were macroscopically parallel to {100} planes and were microscopically dimpled; furthermore, crack growth occurred in <110> directions with extensive slip on {111} planes around crack tips. For the CPH metals, cleavage fractures were macroscopically parallel to basal planes, were also microscopically dimpled in some instances, and crack growth occurred in $<2\bar{1}\bar{1}0>$ directions. These observations suggest that cleavage is not necessarily an atomically brittle process (as often thought) and it is proposed that cleavage can occur by localised plastic flow at crack tips in some materials. It is also suggested that cleavage of normally ductile materials in embrittling environments can be explained on the basis that chemisorption facilitates nucleation of dislocations at crack tips.

KEY WORDS

Cleavage fracture, mechanisms, dislocations, voids, liquid-metal embrittlement, chemisorption, FCC and CPH metals, fractography.

INTRODUCTION

Fracture can involve such extensive deformation that specimens neck down to an edge, or so little deformation that specimens are brittle on an atomic scale. Between these two extremes, there are many cases where fracture involves nucleation, growth and coalescence of voids ahead of cracks so that fracture surfaces are dimpled. When deformation is extensive, dimples are quite large and deep and fractures are macroscopically ductile. However, when deformation is highly localised at crack tips, dimples are very small and shallow and fractures are macroscopically brittle. It is generally accepted that the formation of dimpled fracture surfaces (regardless of dimple size) involves intense dislocation activity around cracks, so that on an atomic scale, crack growth occurs by nucleation or egress (or both) of dislocations at crack tips. For very brittle materials, however, it is generally assumed that crack growth occurs by tensile separation of atoms ('tensile decohesion') at atomically sharp crack tips; in this case, dislocations should not generally intersect crack tips, voids should not form ahead of cracks, and fracture surfaces should be essentially flat on an atomic scale.

Cleavage fracture[1] has usually been considered to occur by tensile decohesion and, hence, proposed criteria for predicting cleavage have been based on the relative stresses required for slip and for decohesion at crack tips. For example, Kelly, Tyson and Cottrell (1967) proposed that the largest shear stress at the crack tip must be less than the theoretical shear strength, when the maximum tensile stress is equal to the stress required for tensile decohesion. Rice and Thomson (1974) suggested that, since the stress is highly localised near crack tips, the stress required for nucleation of dislocations (rather than the theoretical shear stress) should be considered and, hence, they proposed that cleavage should occur when there is a large energy barrier against the emission of dislocations at crack tips. On the basis of such analyses, cleavage is predicted when $\gamma/\mu b \lesssim 0.1$, where γ is the surface energy, μ is the shear modulus, and b is Burgers vector (Tyson, 1977). Gandhi and Ashby (1979) suggested that the ratio σ/K (where σ is the flow strength at 0 Kelvin and K is the bulk modulus) better predicts fracture behaviour. Thus, σ/K (x0.001) averages 0.3 for FCC metals, 0.9 for BCC metals, 1.7 for HCP metals, 2.6 for alkali halides, 4.0 for oxides and 7.0 for covalent and hydrogen-bonded solids, in agreement with known tendencies for brittleness. Claims for the validity of these criteria have also been made on the basis that they predict cleavage in iridium; of the FCC metals, only iridium (σ/K = 0.001) and rhodium (σ/K not known) cleave in inert environments. Cleavage planes should be those for which the surface energy is a minimum, although in cases where some dislocation activity (on planes not intersecting crack tips) accompanies cleavage, it has been suggested (Hecker, Rohr and Stein, 1978; Tyson, Ayers and Stein, 1973) that cleavage planes and directions should be those for which the associated plastic work of fracture is minimised. Accordingly, cleavage should occur on {100} planes in <100> directions for BCC and FCC materials.

For metals in particular, there is good evidence that significant plastic deformation does accompany cleavage: transmission-electron microscopy of thin foils close to fracture surfaces, electron fractography, and X-ray back-reflection and electron-channeling patterns from fractures, all generally show evidence of plastic strain. Furthermore, fracture energies are often much greater than surface energies. Since some plasticity is usually evident, the concept that cleavage is an atomically brittle process has been questioned by Beachem (1976) who suggested that cleavage may occur by localised plastic flow at crack tips. Petch (1968) has also suggested

[1]In the present paper, cleavage fractures are defined as those which appear brittle and are parallel to a low-index crystallographic plane, on a macroscopic scale.

that atomically brittle fracture may be less common than has generally been assumed. Cleavage fracture induced in normally ductile metals by testing in embrittling liquid-metal environments has often been considered to be an atomically brittle process (Kamdar, 1973). However, detailed metallographic and fractographic studies of liquid-metal embrittlement in aluminium and nickel (Lynch, 1977, 1979) showed that, although fracture surfaces were macroscopically parallel to {100} planes, they were microscopically dimpled, and there was extensive slip on planes intersecting crack tips. Lynch therefore proposed that cleavage of aluminium and nickel in liquid-metal environments occurred by alternate-slip at crack tips combined with nucleation and growth of small voids ahead of cracks. In the present paper, cleavage has been studied in iridium (FCC) and zinc (CPH) in inert environments and an Al-Zn-Mg alloy (FCC), cadmium (CPH) and titanium (CPH) in liquid-metal environments, to determine whether crack growth occurs by localised plastic flow or tensile decohesion in these cases.

EXPERIMENTAL PROCEDURE

Materials and environments used were (i) single crystals of very high-purity iridium tested in argon and air at 25°C, (ii) single crystals of high-purity Al6.27%Zn2.94%Mg tested in air at 25°C, liquid gallium at 35°C, and a liquid Bi-Pb-In-Sn-Cd eutectic alloy at 60°C, (iii) cadmium polycrystals (1-10mm grain size) tested in liquid gallium at 35°C, (iv) α-titanium polycrystals (~1mm grain size) tested in liquid mercury at 25°C, and (v) zinc single crystals tested in argon and air at 60°C and -196°C. Specimens were notched, and tested in bending under cyclic and monotonic loading. Orientations of fracture planes were determined from Laue X-ray back-reflection patterns and from directions of slip and twin traces on fractures. Directions of crack growth were established from river lines and striations on fractures; striations, marking the position of the advancing crack front, were produced by either cyclic stressing or abruptly changing the conditions of crack growth.

RESULTS

Iridium in Inert Environments

Orientations of specimens were such that {100} planes were approximately normal to the specimen axis; specimens were tested so that the root of the notch and the bending axis were (a) parallel to <100> directions, and (b) parallel to <110> directions. Crack growth (in argon and air) produced cleavage fractures macroscopically parallel to {100} planes, in agreement with previous work (Hecker, Rohr and Stein, 1978), although local deviations (~10°) from {100} planes were sometimes observed in the present work. When the bending axis (and notch root) were parallel to a <110> direction, crack fronts were parallel to the notch root (Fig. 1(a)), but when the bending axis was parallel to a <100> direction, crack fronts were a zigzag shape with segments at approximately 45° to the notch root (Fig. 1(b)). In other words, crack growth occurred in <110> directions regardless of the orientation of specimens. Examination of fracture surfaces by optical and scanning-electron microscopy revealed numerous steps and a few, widely separated dimples (Fig. 2) which were associated with particles. Transmission-electron microscopy of secondary-carbon replicas revealed details which were probably small, shallow dimples

(~0.05μm diameter) over most of the fracture surface; fine, closely spaced slip traces, as well as some coarse slip steps, were also evident (Fig. 3). No such details were observed on surfaces which were extremely flat, e.g. fracture surfaces of glass (Fig. 3(inset)). Laue patterns (from iridium) of fracture surfaces were very diffuse compared with those from strain-free (electropolished) surfaces (Fig. 4) indicating that considerable localised plasticity had occurred during fracture. Observations on the side surfaces of specimens during crack growth also showed that extensive slip had occurred, although little slip was observed directly ahead of cracks (Fig. 5).

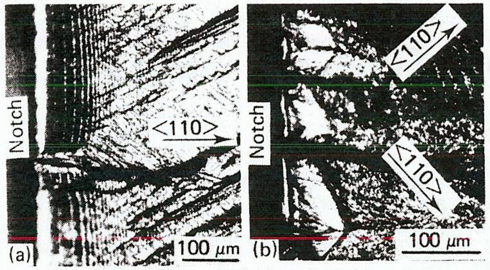

Fig. 1 Optical micrographs of fatigue striations in Ir.

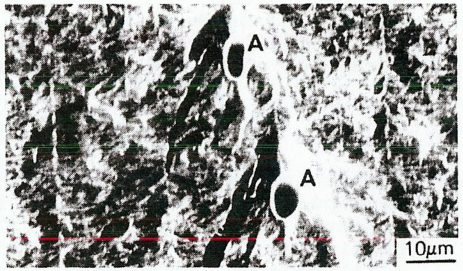

Fig. 2 SEM of cleavage in Ir showing dimples (A) and steps.

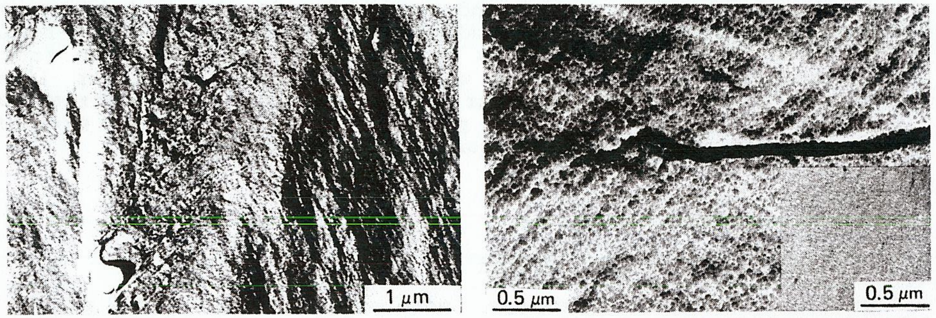

Fig. 3 Replicas of cleavage in Ir showing very small dimples and fine slip traces, and (inset) fracture surface of glass.

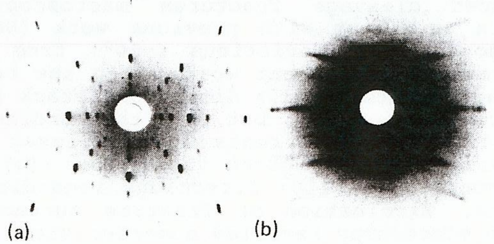

Fig. 4 Laue patterns for (a) strain-free {100} surface and (b) {100} fracture surface.

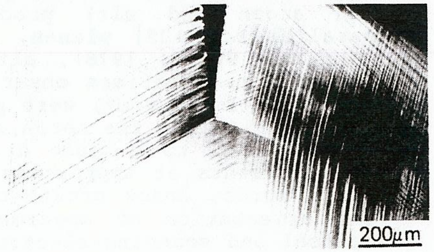

Fig. 5 Optical micrograph of slip around cleavage crack in Ir on the side of a specimen.

Al-Zn-Mg in Liquid-Metal Environments

A variety of crystal orientations and heat-treatments were tested and results were, in many respects, similar to those for iridium. In all cases, crack growth in liquid-gallium and liquid-alloy environments produced cleavage fractures which were macroscopically parallel to {100} planes, except for small deviations (~10° from {100}) in some areas. Crack growth always occurred in <110> directions and, for some specimens, adjacent regions cracked in two <110> directions so that zigzag crack fronts were observed (Figs. 6(a),7). Figure 6 also shows a transition from cleavage fracture in the liquid-alloy environment to 'ductile' fracture in air. Both regions were entirely dimpled but dimples in the cleavage region were much shallower than those in the ductile region (Fig. 6(b),(c)). The size and spacing of dimples (for cleavage and ductile fractures) depended on the specimen heat-treatment and varied in a manner which was consistent with nucleation of voids by aging precipitates ahead of cracks. Laue spots from fracture surfaces were quite diffuse and it was estimated (by comparison with Laue patterns from specimens given known amounts of strain) that strains just beneath fracture surfaces were ~50% in some cases. Observations on the side surfaces of specimens during crack growth showed that the slip distribution was similar to that observed for iridium, i.e. slip occurred particularly on {111} planes intersecting the crack-tip region. Moreover, for Al-Zn-Mg, the slip distribution in the specimen interior (Fig. 8) (revealed by aging partially cracked specimens, then sectioning, polishing and etching) was similar to that at the surface. Details of these results are to be published elsewhere.

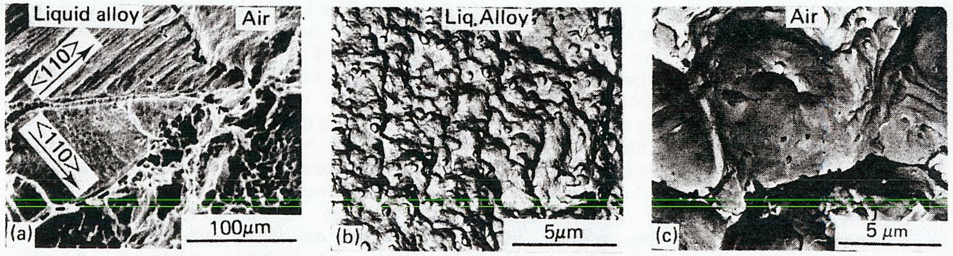

Fig. 6(a) SEM showing transition from cleavage to ductile fracture in overaged Al-Zn-Mg, (b) and (c) TEM (replicas) of cleavage and ductile regions, respectively.

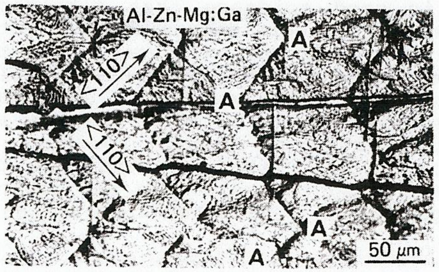

Fig. 7 Optical micrograph of fatigue striations (A-A) for Al-Zn-Mg in liquid Ga.

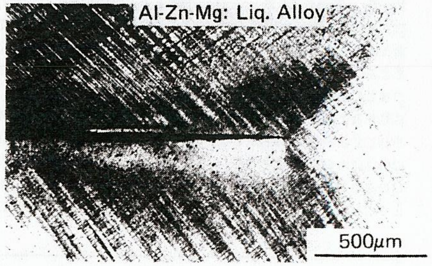

Fig. 8 Optical micrograph of slip around cleavage crack in Al-Zn-Mg in specimen interior.

Cadmium and Titanium in Liquid-Metal Environments

Fracture of polycrystalline cadmium and α-titanium (which are ductile in inert environments) in liquid gallium and liquid mercury, respectively, produced reflective cleavage facets which were generally macroscopically parallel to basal planes (Fig. 9(a,b)). River lines and twin traces were evident and the directions of river lines suggested that crack growth occurred in $\langle 2\bar{1}\bar{1}0\rangle$ directions. Electron fractography showed that cleavage facets were dimpled in many areas (Fig. 10(a,b)). Most dimples were quite small and shallow although, for α-titanium, quite large, elongated dimples ('flutes') were also observed in some areas. Compared with the FCC metals, Laue patterns from fracture surfaces were fairly sharp, and only a small amount of slip was observed on the side surfaces of specimens around cracks.

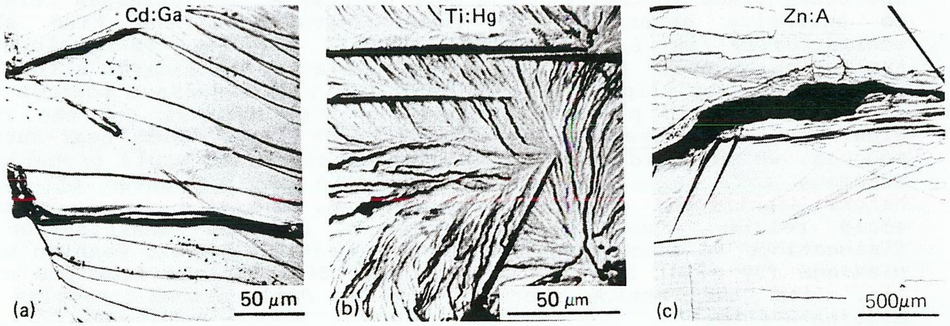

Fig. 9 Optical micrographs showing cleavage facets for Cd, Ti and Zn.

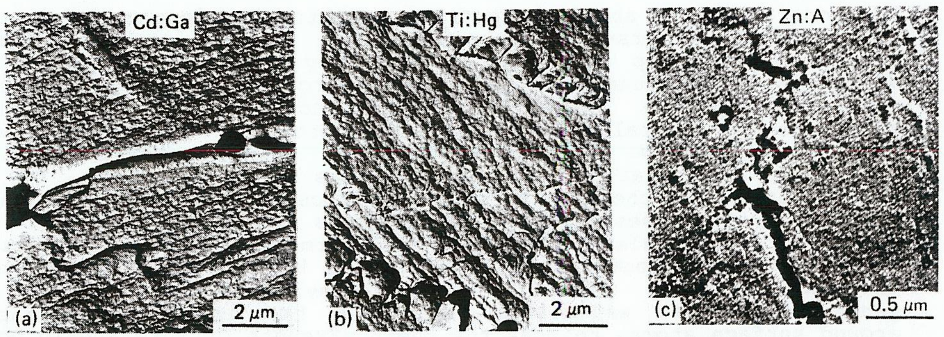

Fig. 10 Replicas of cleavage facets for Cd, Ti, and Zn.

Zinc in Inert Environments

Cleavage of zinc was macroscopically similar to cleavage in cadmium and α-titanium in liquid-metal environments in that fracture surfaces were parallel to basal planes and crack growth occurred in $\langle 2\bar{1}\bar{1}0\rangle$ directions (Fig. 9(c)). On a microscopic scale, for fractures produced at 60°C, replicas revealed fine details which were possibly extremely small dimples (Fig. 10(c)), but for fractures produced at -196°C replicas showed comparatively little detail.

DISCUSSION

Atomic Mechanisms of Cleavage

For the FCC metals, the main assumptions and predictions of theories envisaging atomically brittle cleavage were not substantiated by the present observations. The observations suggested that voids formed ahead of cracks and that extensive slip intersected crack tips during cleavage. Moreover, crack growth occurred in $\langle 110\rangle$ directions 45° from the $\langle 100\rangle$ direction predicted by Hecker, Rohr and Stein (1978), even when the applied bending stress favoured a $\langle 100\rangle$ direction. Small voids ahead of crack tips cannot be observed directly, but it is generally accepted that formation of dimpled fracture surfaces involves nucleation and growth of voids ahead of cracks. Nucleation and growth of voids generally involves intense, local dislocation activity, and it was evident from the diffuse Laue patterns from fracture surfaces that such activity had occurred. Furthermore, the occurrence of slip extending some distance from the crack tip on planes intersecting (or nearly intersecting) crack tips suggests that slip exactly intersects crack tips since the shear stress should be greatest exactly at crack tips. Thus, the stresses around crack tips are probably relaxed by slip before the stress required for tensile decohesion is attained.

The nucleation and subsequent movement of dislocations from crack tips on two intersecting $\{111\}$ slip planes, alternately, would produce crack growth in the observed $\langle 110\rangle$ directions since $\langle 110\rangle$ directions are normal to the line of intersection of $\{111\}$ slip planes. Furthermore, the coalescence of cracks growing by alternate-slip with voids, associated with deformation ahead of cracks, would account for small dimples and fine slip traces on fracture surfaces macroscopically parallel to $\{100\}$ planes (Fig. 11) (Lynch, 1979). An alternate-slip process probably occurs because, if more dislocations were emitted on one side of the crack than the other, then a larger back-stress opposed to subsequent slip would counteract further dislocation nucleation on the more active side. Thus, it is concluded that cleavage in FCC materials can best be explained in terms of localised plastic flow rather than decohesion.

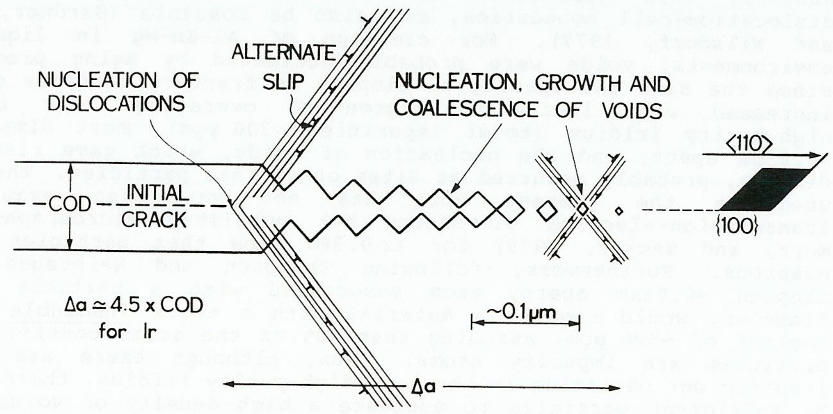

Fig. 11 Alternate-slip/void-growth mechanism for cleavage in Ir.

Similarly, cleavage in CPH metals could be explained by alternate-slip on {11$\bar{2}$2} planes intersecting crack tips combined with void formation ahead of cracks. Such a process would produce dimpled fracture surfaces macroscopically parallel to basal planes, and crack growth in <2$\bar{1}\bar{1}$0> directions, as observed in the present work for cadmium, titanium and zinc at 60°C. For cleavage of zinc at -196°C, no dimples were observed; however, it is possible that there were dimples which were so small and shallow that they were not detected. Plasticity around cracks produced by an alternate-slip/void-growth mechanism could also be difficult to detect in some cases since dislocations nucleated at crack tips probably have to move only small distances to contribute to crack growth. Thus, for cleavage of zinc at -196°C, it is not obvious whether crack growth occurs by an alternate-slip/void-growth process or a tensile decohesion process (accompanied by an atmosphere of dislocations which do not generally intersect crack tips). For BCC metals (not studied here), cleavage on {100} planes could also possibly occur by alternate-slip (on {112} planes) at crack tips with nucleation and growth of voids ahead of cracks. Crack growth should then occur in <110> directions (as for FCC metals) and published micrographs (Hull and Beardmore, 1966) of cleavage fractures in tungsten single crystals show that river lines and, hence, probably crack growth are generally parallel to <110> directions. Thus, cleavage by a localised plastic flow process could be quite common for metals and further studies to differentiate between tensile decohesion and slip mechanisms of cleavage in other materials would be worthwhile.

Nucleation and Growth of Voids

The formation of voids ahead of cracks is an important feature of the proposed cleavage mechanism since alternate-slip, by itself, would produce extensive opening of the crack as well as crack growth, and would probably eventually lead to general yielding (Cottrell, 1965). Nucleation of voids ahead of cracks generally occurs in regions where plastic deformation is markedly inhomogeneous and separation of particle/matrix interfaces or fracture of brittle particles is usually involved (Goods and Brown, 1979; Thompson and Weihrauch, 1976.) However, void nucleation at sites other than particles, e.g. dislocation-cell boundaries, may also be possible (Gardner, Pollock and Wilsdorf, 1977). For cleavage of Al-Zn-Mg in liquid-metal environments, voids were probably nucleated by aging precipitates since the size and spacing of dimples on fracture surfaces generally increased with increasing degree of overaging. For the very high-purity iridium (total impurities <300 ppm), most dimples were ~0.05μm apart, and the nucleation of voids, which gave rise to the dimples, probably occurred at sites other than particles. The iridium used in the present work has not yet been examined by transmission-electron microscopy but published micrographs (Rohr, Murr, and Hecker, 1979) for Ir 0.3%W show that particles are not numerous. Furthermore, following Thompson and Weihrauch (1976), dimples ~0.05μm apart, each associated with a particle ~0.005μm diameter, would require a material with a total insoluble impurity content of ~500 ppm, assuming that 50% of the atoms constituting the particles are impurity atoms. Thus, although there are probably insufficient particles in the very high-purity iridium, there may well be sufficient particles to nucleate a high density of voids in many 'pure' materials such as the cadmium, α-titanium and zinc used in the present work.

Criteria for Cleavage

On the basis of the foregoing results and discussion, it is proposed that 'ductile versus brittle behaviour' depends on which of (i) tensile decohesion at crack tips, (ii) nucleation and movement of dislocations from crack tips, or (iii) extensive dislocation activity ahead of crack tips, predominates when a cracked solid is stressed. Tensile decohesion at crack tips, before either dislocations nucleate at crack tips or large strains develop ahead of cracks, would obviously result in atomically brittle behaviour. However, macroscopically brittle behaviour should also result if crack growth occurs readily, compared with extensive general slip ahead of cracks, regardless of the mechanism of crack growth. Thus, if dislocations nucleate and subsequently move from crack tips (on slip planes >90° to the crack plane so that crack growth occurs) at low stresses relative to extensive general slip, then cleavage of the kind shown schematically in Fig. 11 could occur. However, if dislocation nucleation at crack tips was difficult relative to general slip, then crack growth (by slip) would not occur until near-surface sources were activated on slip planes which were greater than 90° to the crack plane and which exactly intersected crack tips. Such near-surface sources, which could be activated at low stresses, would probably be uncommon and, hence, large strains would develop ahead of cracks before significant crack growth occurred, i.e. 'ductile' fracture would result. Thus, ductile fracture involves annihilation of dislocations at crack tips probably in a rather chaotic fashion while cleavage (by slip) involves injection of dislocations from the crack tip, and interaction between these dislocations results in alternate-slip.

The considerations above suggest that, if tensile decohesion does not occur, ductile versus brittle behaviour depends on the relative proportions of slip on planes intersecting crack tips compared with general slip around cracks—larger proportions of the former favouring brittle behaviour. For ductile metals in inert environments, general slip predominates, probably because (i) five or more slip systems readily operate at low stresses, and (ii) dislocation nucleation at crack tips is inhibited by the non-uniformity of the lattice at the surface (Fleischer, 1960). (This non-uniformity arises because surface atoms have fewer neighbours than those in the bulk.) Cleavage in normally ductile metals in liquid-metal environments could therefore be explained on the basis that chemisorption (the only material-environment interaction that generally occurs) effectively increases the number of neighbours around surface atoms, reduces the shear strength of interatomic bonds, and facilitates nucleation of dislocations at crack tips (Lynch, 1977; 1979). In inert environments, cleavage (by slip) may occur because there are either a limited number of operative slip systems (e.g. some CPH metals), or a high inherent resistance to slip and high rate of work-hardening (e.g. Ir), so that the stress required for dislocation nucleation at crack tips is attained before large strains develop ahead of cracks. A high resistance to slip and high rate of work-hardening probably inhibit the development of a general strain ahead of cracks to a greater extent than crack growth by slip since the former requires extensive dislocation activity in a reasonable volume of material while the latter requires dislocation nucleation and subsequent movement over relatively short distances from crack tips. The characteristics of clean surfaces (in inert environments) probably varies from material to material so that dislocation nucleation at surfaces and, hence, the propensity for cleavage also varies. The last factor is not well understood and, judging from the effects of liquid-metal environments on fracture, is obviously very important.

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