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Importance of dislocation cores in fatigue fracture

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Abstract It is pointed out that proposed mechanisms of fatigue fracture should be consistent with Coffin's Law for constant strain-amplitude cyclic deformation. Most proposed mechanisms are not. The fracture of dislocation cores along their glide planes is consistent with the fact that the law describes the behavior during the first ¼ cycle as well as that after a very large number of cycles. Experimental evidences of the relative weakness of edge dislocation cores is described. Analysis of this weakness by Bullough, and in this article, discussed. It is concluded that this effect plays an important role in fatigue fracture.

Introduction

Coffin's law of the fatigue failure of metals applies equally to a tension test (single ¼ cycle), or to a very large number of deformation cycles. The law (originally discovered by Liu et al., Fig. 1) states that if the deformation amplitude is $\Delta\delta$ during deformation cycling, then the number of cycles to failure, N_f, is inversely proportional to the square of the amplitude. That is:

$$N_f = \text{const.}(\Delta\delta)^{-2}. \tag{1}$$

Coffin observed that, for a large number of metals and alloys, this equation is obeyed from ¼ to as many as 10^6 cycles. This remarkable observation means that the mechanism of failure is present during the first ¼ cycle, but does not cause immediate failure if the deformation amplitude is reduced. Many deformation cycles are needed for failure at reduced amplitudes.

A single simple causative parameter-like deformation amplitude is unlikely to have complex consequences that develop progressively with its repeated application. In this case, the evidence is that the causative parameter is present already during the first ¼ cycle. That is, it is not something that develops during repeated cycling such as intrusions or extrusions. They do develop, but as a secondary phenomenon; not as the primary cause of fatigue failure.

Because plastic deformation is mediated by the motion of dislocation lines, and the line length follows first-order kinetics, the concentration of dislocations increases linearly with the amount of plastic deformation. When the deformation is cyclic, the dislocation density partially decreases during the cycle reversals (the Bauschinger effect), but it increases monotonically with the integrated deformation. Thus, it may be concluded that it is the dislocations themselves that lead to fatigue failure.

During a tension test (¼ cycle), a large stress level must be reached before fracture occurs because isolated individual dislocations cause relatively little weakening. However, during cyclic deformation, as dislocations accumulate in a material they cause increasing weakening just as one small slit in a piece of paper causes little decrease in its strength, but a row of slits causes a considerable decrease.

Elastic versus inelastic effects of dislocations

Plastic shear bands act like shear cracks causing elastic stress concentrations [1]. However, such stresses are limited by the plastic flow stress in a material, so they usually do not become large. They have been blamed for many

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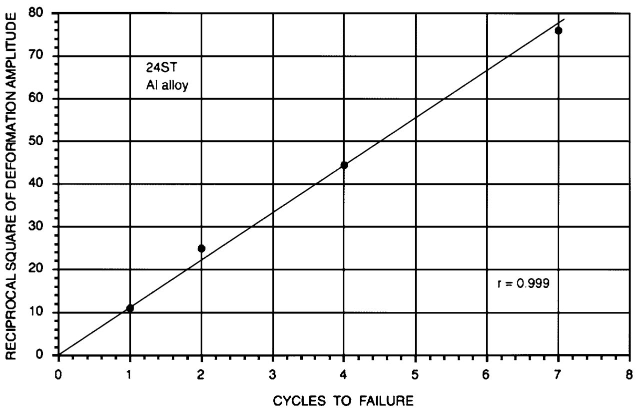


Fig. 1 Early data demonstrating Coffin's law [16]

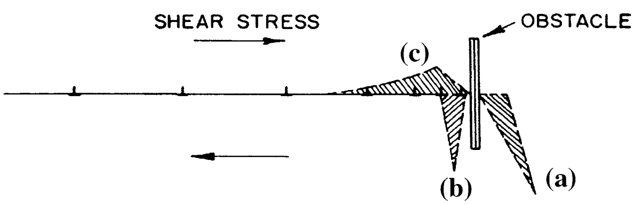


Fig. 2 Possible positions of cracks in concentrated stress region at tip of dislocation "pile-up"

fractures in materials, but there is no direct evidence because if a crack forms the evidence is destroyed. Fractures inferred to have been caused by the elastic stress fields of dislocations were reviewed comprehensively by Stroh [2, 3]. In his case the cracks lay perpendicular to the glide planes. They lie parallel to the glide planes in the present discussion (Figs. 2 and 3), so much of the previous analysis is not pertinent.

The material within the cores of dislocations behaves inelastically. Because of the decreased atomic density there the local cohesion is reduced. In the case of edge dislocations, the core configurations resemble incipient slits. These slit-like configurations have been discussed within the context of elasticity theory by Yoffe [4], but their inelasticity was not considered.

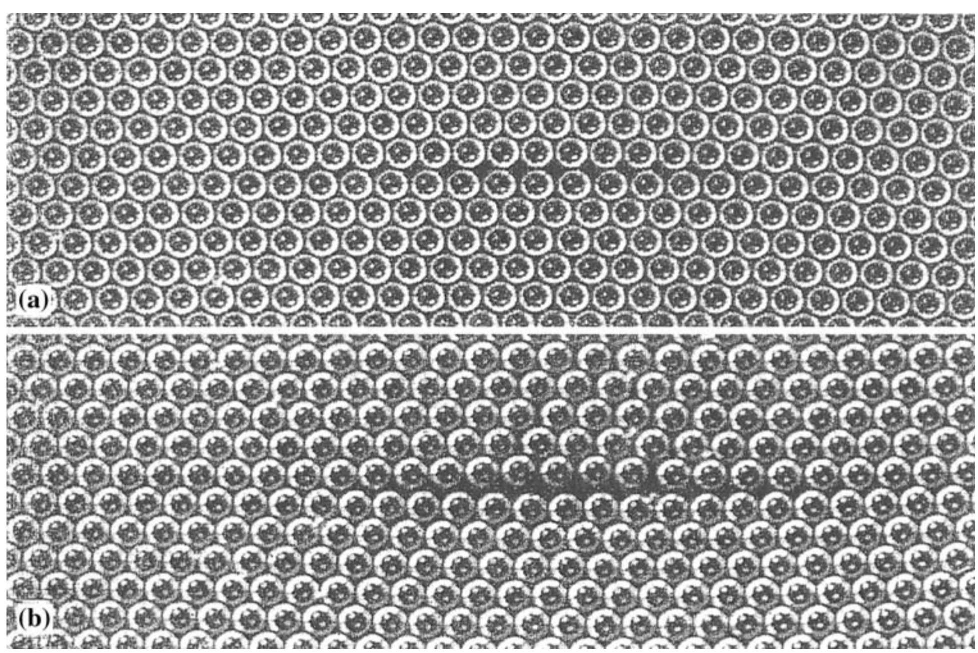
The first evidence that elasticity theories are inadequate came from experiments of Deruyttere and Greenough [5] who studied the variation of the fracture stress of zinc crystals with the angle, χ between the (0001) planes and the tension axis. They found a minimum fracture stress at χ equal about 45° rather than 90°, indicating that prior plastic deformation has a large effect on the fracture stress. This was soon followed by experiments of Gilman [6] that confirmed the previous experiments, and provided further evidence that dislocations on glide planes reduce their fracture strengths.

Analysis by Bullough [7] succeeded in rationalizing the observations of Deruyttere and Greenough as well as those of Gilman. His analysis was based on continuous distributions of infinitesimal dislocations. Thus it was an elastic analysis with an improved configuration, but did not explicitly deal with the inelasticity of the dislocation cores.

Experimental evidence of the weakness of dislocation cores

In addition to the evidence of Deruyttere and Greenough, and of Gilman, already cited, there are other experimental results showing that edge dislocation cores are relatively

Fig. 3 Bubble rafts: (**a**) dislocation at center with no applied stress, (**b**) cracking of dislocation core under applied tension



weak in tension. They include: behavior of bubble rafts, unbending of bent zinc crystals, cleavage of prestrained LiF crystals, unbending of bent steel bars, tension applied to pre-twisted bars, and more.

Bubble model

Direct general proof of the weakness of edge dislocation cores is given by the behavior of bubble rafts. Although these rafts are not metal crystals, Bragg and Lomer [8, 9] showed that rafts with appropriate bubble sizes mimic the mechanical properties of metal crystals, so they are reasonable models.

Edge dislocations in bubble-raft crystals are unstable to tension applied perpendicular to their glide planes. Tension splits them open. The tension can be applied easily by creating waves in the liquid that supports the bubbles. When the crest of a wave, whose velocity vector is normal to a dislocation's glide plane passes through the core of the dislocation it puts it in tension. Figure 2 from Gilman [6] shows this. The applied stress in this case is quite large.

Cracking at dislocation cores in bubble rafts proves that the cores are relatively weak. If only one is present a material remains relatively strong, but if they accumulate, they can cause fracture under relatively small stresses. Similarly, as mentioned above, a single small slits in sheets of paper causes little weakening, but a row of slits cause considerable weakening.

Zinc bicrystals

In zinc crystals the cleavage plane is (0001). This is also the primary glide plane. In zinc bicrystals, after some plastic deformation has occurred, fracture begins at the grain boundaries on (0001) planes (i.e., parallel to the glide planes). Assuming that obstacles such as grain boundaries cause dislocations to pile-up and thereby cause a concentration of stress, there are various possibilities for crack formation. These are illustrated in Fig. 2. Koehler [10] proposed that a crack should form as at (a) in the figure. Zener [1] and Stroh [2, 3] proposed case (b). Bullough [7] suggested case (c) as observed in zinc. Gilman [6] agreed with Bullough, stating: "dislocations may be considered to be stable but subcritical Griffiths cracks which can become critical in size in the presence of concentrated stresses." Calculations showed that measurements on zinc are consistent with this view, but proof is lacking because critical cracks (by definition) cannot be observed.

Curved zinc crystals

An excess of edge dislocations of a single sign causes bending of the glide planes in crystals [11]. Since zinc has a single primary glide plane, it shows this effect clearly (Fig. 4). If the bending moment used to cause the bending is then reversed, it is observed that the crystals have become brittle [12]. Bent crystals cannot be straightened if the curvature has exceeded a critical value (Fig. 4). That is, if the excess dislocation density reaches a critical value.

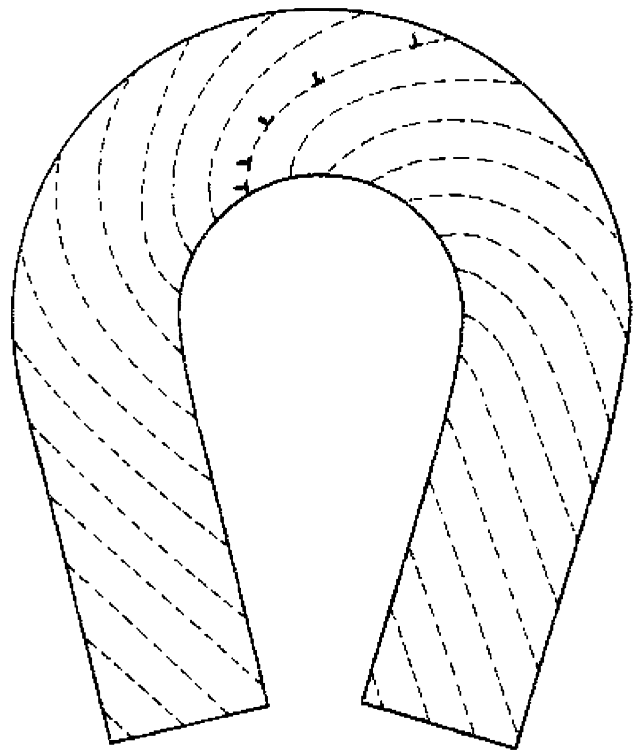


Fig. 4 Schematic illustration of the curved glide planes in a bent zinc crystal

It was found experimentally, for about 24 zinc crystals with various amounts of bending, that the excess dislocation density times the tensile fracture stress was constant. Since the distribution of the excess dislocations on and among the glide planes was not known, the stress per linear density along the glide planes could not be determined, but it was found that a clear correlation between dislocation density and strength exists.

Since the dislocations in the bent crystals were not subject to concentrated stresses (little, if any, "piling up"), the behavior may be interpreted to mean that the cores of the excess dislocations themselves weaken the glide planes.

Cleavage after prestrain

LiF crystals can be readily cleaved, provided they are not too pure (i.e., too soft). The cleaved surfaces of as-grown crystals are quite flat (mirror like). However, if a crystal is plastically compressed prior to cleavage, the cleaved surfaces become slightly rough and many microscopic branch cleavages are observed on the (110) glide planes that

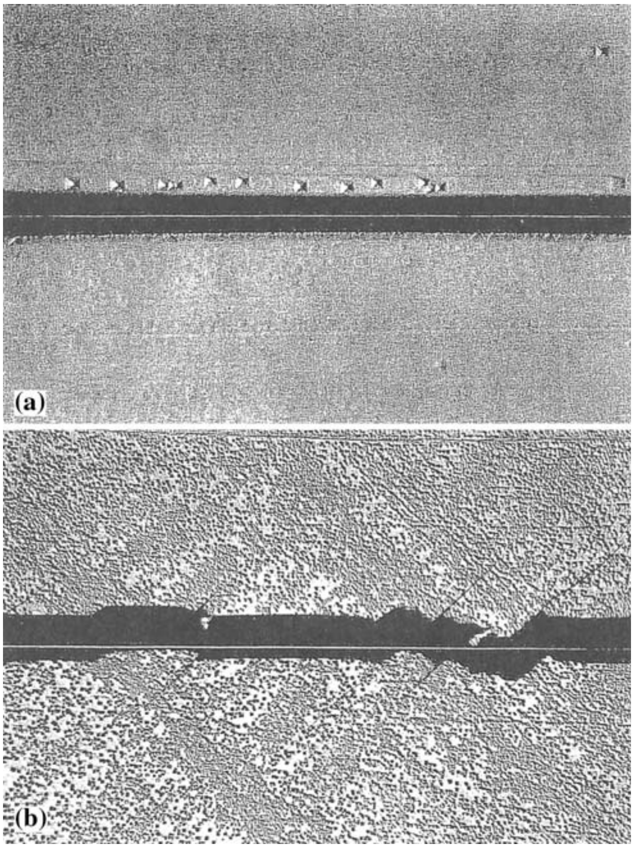


Fig. 5 Photographs of cleaved LiF crystals (both specimens etched to show positions of dislocations): (**a**) side view of cleavage crack in an as-grown crystal, (**b**) cleavage crack edges in crystal compressed 3% at room temperature prior to cleavage at 78 K followed by etching

intersect the (100) cleavage planes [13] (see Fig. 5). These are revealed by cleaving the specimens at right angles to the initial cleavage plane to show the cross section. When such cross sections are etched to show where the dislocations caused by the plastic compression are, it is found that branching cleavages lie on the formerly active glide planes. This shows that plastic deformation has weakened these planes. Note that the deformation-induced cleavage occurs on the (110) glide planes, not on the (100) cleavage planes. This is strong evidence that glide dislocation cores have weakened the glide planes.

Plastic twisting prior to tensile fracture

If a cylindrical bar of a semi-ductile material is plastically twisted and then subjected to axial tension, it is found to be weakened by the prior twisting. This suggests that relatively weak glide planes are introduced by the twisting which introduces crossed grids of screw dislocations. The phenomenon is sometimes called "slip-band decohesion." It suggests that screw dislocation cores may also be centers of weakness.

Twisting polycrystalline specimens involves relatively complex processes. However, a simple experiment could be done that would be quite unambiguous. A zinc crystal oriented with its <0001> axis parallel to its cylindrical axis could be twisted and then fractured in tension. The screw dislocations densities in such specimens would be proportional to the torsional deformation (and any edge components would lie along the (0001) planes). Thus the weakening effect of screw dislocation cores could be quantified experimentally.

Reversal of bending

If a mild steel bar is severely bent (into the shape of a horseshoe) and then forces are applied to straighten it, it often breaks (consistent with Coffin's law). During this third-quarter cycle, "pileups" or other stress concentrations are being relieved, so this does not appear to be an elastic effect. A straightforward conclusion is that the strength of the material has been reduced during the initial bending; especially toward a reversal of the sign of the applied stress.

Severe plastic bending puts into the steel a large concentration of edge dislocation dipoles (testified by the deformation hardening) plus an excess of dislocations of one sign to accommodate the bending. It seems reasonable to expect that aggregations of these dislocations cause the embrittlement.

Analysis of core weakness

A rigorous quantum-mechanical analysis of the change in cohesion at the core of a dislocation is not feasible. Bullough's analysis is a reasonable approximation, and another approximate type of analysis will be presented here. Since the normal crystal structure is disturbed at a core, there is no doubt that the local cohesion is decreased. The question is: how much? And, how many cores must be aggregated to create the equivalent of a super critical crack under a given applied stress?

In order to estimate the amount of weakening at a dislocation core, the local energies are considered. This treatment is only approximately correct. At the center of an edge dislocation core, there are large shears which affect any covalent bonding. However, metallic bonding is only weakly dependent on shear deformation, so the shears will be ignored. The maximum change in volume (strain) occurs at the core center. This is relatively small, however, so linear behavior will be assumed. The model is slit-like, analogous to elastic case analyzed by Yoffe [4].

The 2D slit-like region at the dislocation core can be described by a displacement field (Fig. 6):

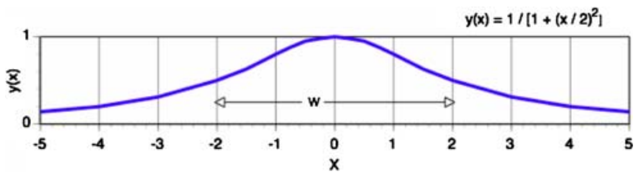


Fig. 6 Shape of schematic slit used for dislocation core-crack model

$$y(x) = y_M[1 + (x/2)^2]^{-1} = y_M[1 + \alpha^2 x^2]^{-1}, \quad (2)$$

where y is perpendicular to the glide plane and x lies in the glide plane. y_M is the maximum displacement. α = width parameter = ½ in Fig. 6. The undisturbed distance between the top and bottom of the glide plane is a. Then, the local strain is: $(y/a - 1)$ and the strain energy density, $u(x)$ [in terms of the maximum strain = $(y_M/a) - 1] = \varepsilon_M$] is approximately:

$$u(x) = (Y/2)\varepsilon_M^2 = \text{Const.}/[1 + \alpha^2 x^2]^{-2}, \quad (3)$$

where Y is the Young's modulus. The integral of this from $-\infty$ to $+\infty$ gives the total strain energy:

$$U = \text{Const.} \int [1 + \alpha^2 x^2]^{-2} dx = \text{Const.}(\pi\alpha/2\sqrt{2}) = Y\varepsilon_M^2(\pi/2^{5/2})\alpha = 0.56\alpha Y\varepsilon_M^2. \quad (4)$$

The maximum strain is about: $1 - (1/2)\sqrt{3} = 0.134$, so $\varepsilon^2 = 0.018$. For the case of iron, $Y = 200$ GPa. so if $\alpha = 0.5$, $U = 1.06$ GPa. Then, if the slit is taken to be two atoms = 5.12 Å wide, the equivalent surface energy of the top and bottom of the slit is 540 mJ/m^2. This is roughly one-third of the surface energy of iron. Thus edge dislocation cores do indeed cause considerable weakening.

Another method for making an estimate is to consider the effect of the change of electron density in an edge dislocation core. The glide plane of an edge dislocation is like an internal surface so plasmons may be trapped there as they are at free surfaces. There is some experimental evidence for this from electron microscopy [14]. Although the change in three-dimensional electron density is small at a dislocation core, the two-dimensional density change is significant. The fractional change in plasmon energy, U, with change of electron density, n, is given by:

$$(\Delta U/U) = (1/2)(\Delta n/n). \quad (5)$$

Taking aluminum as an example, the plasma energy is 10.3 eV, and the surface energy is 900 erg/cm^2 $\approx$ 0.5 eV/atom, so a 5% change in electron density corresponds to the fracture surface energy.

Damage accumulation

As plastic deformation proceeds, relatively stable dislocation dipoles, and other multipoles form so dislocations accumulate in proportion to the amount of deformation, and a material becomes progressively weaker. Individual cores collect into arrays. These arrays (persistent slip bands) have effective widths, w_{eff} which increase with the plastic deformation, δ. This effect is similar to a string of small cracks that weakens a material more than a single crack [15]. The width of such a string can become large enough to reach the Griffith instability condition.

For cyclic deformation, the dependence of w_{eff} on δ may be small because relaxation occurs during the reversal part of each cycle. However, w_{eff} can be estimated from Coffin's Law.

Summary

It is argued both by induction and deduction that the weakness of the cores of edge dislocations plays an important role in fracture phenomena. This weakness of the cores (increase in the local energy) is a result of the disturbance of the crystal structure in these cores. Its magnitude is estimated from a slit model of a core applied to iron. Several experimental observations support the idea that dislocation cores are weak relative to perfect crystal structures.

Dislocation core weakness, unlike other proposed mechanisms, is consistent with Coffin's law, so it appears to play an important role in fatigue fracture.

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