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Cracks and extrusions caused by persistent slip bands

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Cottrell's account of persistent slip poses a puzzle which has challenged all subsequent research. Persistent slip bands (PSB) endure repeated plastic shear which constantly produces narrower and narrower dipoles, as observed by Veyssière. At the same time, because narrow interstitial dipoles have a larger elastic energy than otherwise identical vacancy ones, shear will eject larger interstitial dipoles to the surface, whilst retaining smaller vacancy ones in the interior, thereby producing excess vacancy loops. This causes a longitudinal tensile stress (the 'fibre stress') inside the band. The ejection process lowers the energy by a term linear in the fibre stress, but increases it by a term quadratic in the fibre stress, giving rise to an equilibrium value of the fibre stress, tensile, in order-of-magnitude agreement with observations of extrusions at low temperatures, where only plasticity can occur. The fibre stress produces logarithmic infinities in the surface stress at the edges of the PSB, and thus can be responsible for sharp stage I fatigue cracks. At higher temperatures which allow pipe diffusion and/or volume diffusion, interstitial loops are drawn by the tensile fibre stress into the PSB. Then, as cyclic plasticity attempts to maintain equilibrium, the loops are ejected where the band meets the surface, producing growing extrusions. Such extrusions can grow almost without limit. At low temperatures, the rate of extrusion formation is maximal at one Burgers vector per cycle, but it will be slower than this if it is diffusion limited.

Keywords: cracking; cyclic deformation; dislocations; fatigue; mechanical behaviour; metallic alloys; plasticity of metals; slip bands

1. Introduction

Failure of rotating machinery, such as axles for railway carriage wheels, initiated research into metal fatigue. The great pioneer 150 years ago was August Wöhler, who introduced the concept of the fatigue limit, the alternating stress amplitude below which failure would not occur. Failure of the Comet jetliners in the 1950s prompted a renewal of research into the fundamentals of crack initiation and growth in metals subjected to repeated cycles of loading and unloading. The extensive literature can be roughly classified into two groups: the engineering group, concerned with crack propagation; and the atomistic group, concerned with mechanisms of initiation at otherwise smooth surfaces.

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In the former group, perhaps the most important and useful papers are those concerned with the 'Coffin-Manson' relation between the imposed plastic strain amplitude and the number of cycles to failure [1,2]. Under stress control, there is the 'Paris law' [3,4], a semi-empirical power-law relationship between the imposed alternating stress intensity and crack growth. Such work assumes that cracks pre-exist in engineering structures, and that what matters is to assess structural integrity by quantifying crack growth. The relevant literature deals in various ways with a problem, sometimes called the 'short crack problem' [5]. Contrary to power-law analysis of crack growth, there is a threshold stress-intensity for pre-existing 'long' cracks. The measured threshold is about a factor of three larger than that expected for the growth of an ideally brittle 'Griffith' crack, a limit which gives a growth rate of less than one atomic spacing per cycle [6]. Contrary to this, some very short cracks, less than a few microns in length, grow unexpectedly rapidly. Cracks initiate from the surface and grow at sub-threshold stress intensities. The Paris law predicts zero growth for a crack of zero length, and clearly fails for initiation and growth at smooth surfaces [7]. The Coffin–Manson relation greatly overestimates the number of cycles to failure when the plastic strain amplitude is small. Despite these shortcomings, it seems that power-law methods of dealing with cracks in working engineering structures are of wide utility. The methods rely crucially on effective methods for detection of small cracks.

The latter group of papers concerns crack initiation. Striking observations of extrusions associated with cracks were made by Forsyth [8,9]. Explanations soon followed. Notably they include May [10], who proposed that cracks are the result of random in-and-out slip steps at surfaces, a model which emphasised the close relationship between plasticity and crack initiation, a relationship clear since the pioneering metallographic observations of Ewing and Humfrey in 1903 [11]. Mott [12] suggested a mechanism based on the systematic cross-slip of screw dislocations to produce an extrusion at the surface and a vacancy loop in the interior, thereby proposing an intimate relationship between dislocation cross-slip, extrusions and crack initiation. Mechanisms based on systematic participation of secondary slip systems in the back-and-forth motion of primary dislocations were also proposed by Cottrell and Hull [13] and more recently by Lynch [14]. A fuller assessment of these ideas is to be found in the books by Frost, Marsh and Pook [15] and by Klesnil and Lukas [16]. It is of great interest that each of the proposed mechanisms captures an important aspect of the puzzling behaviour.

The basic problem is most succinctly and accurately expressed in Cottrell's book 'The mechanical properties of matter' [17], section 11.11. Anyone seeking to understand crack initiation cannot do better than to read this. What follows is a selective quotation, accompanying Figure 1, reproduced from Cottrell's book:

"Oscillating slip bands in internal grains do not seem to produce fatigue cracks. A free surface, usually the external surface, appears to be necessary, probably as a place to deposit material pushed out of active slip bands to make space for cracks. This may be why sharp, deep notches have less effect on fatigue strength than elasticity theory would suggest. Active slip lines which meet the surface behave quite remarkably. Thin tongues of material, called *extrusions*, grow rapidly out of them, and at the same time, narrow crevices, called *intrusions,* spread down them into the body, as shown in Figure 1. Extrusions and intrusions have been seen on many materials, under various conditions. In a long fatigue test they usually form during the first 5–10% of the fatigue life. The exact manner of their formation is still not established. They may form by a

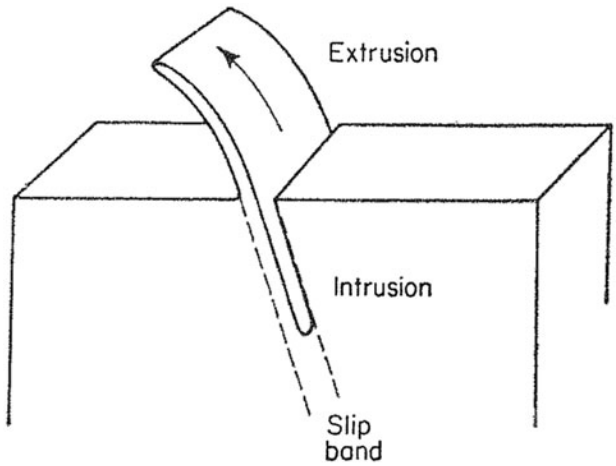

Figure 1. Shows the salient features of extrusion and intrusion formation in Cottrell's characteristic clear and uncluttered way. It is Figure 11.19 from A. H. Cottrell, *The Mechanical Properties of Matter*, [17], now sadly out of print (Figure reproduced with permission from Dr. G. A. Cottrell.) Modern studies show that the 'intrusion' is a sharp crack, found usually on the side of the extrusion opposite to that depicted.

process in which oscillating dislocations do not precisely retrace their path up and down the slip plane but jump from one face of the plane to another, e.g. by cross-slip, at the ends of their path. Alternatively, they may form simply statistically, by random slips on a packet of planes, so that by chance some planes glide out of the packet. A third possibility is that soft material in the slip bands is squeezed out plastically during the compressive phase of the cycle and not sucked back in again during the tensile phase …

… There seems little doubt that the fatigue crack starts from an intrusion (or in some cases a similar notch formed along a grain boundary). As it spreads down the slip band into the material, the incipient fatigue crack slows down and at a depth of $10^{-3} \rightarrow 10^{-2}$ cm becomes almost 'dormant'. In tests lasting $10^6 \rightarrow 10^7$ cycles, over three-quarters of the total fatigue life may be spent in this dormant phase. If the applied stress is sufficiently small … the crack may even cease growing altogether (*non-propagating fatigue cracks*). What happens during the almost dormant stage of growth is not yet understood … "

2. A current perspective

Since the work outlined in the introduction, very substantial progress has been made. It is now established that repeated cycling at controlled plastic strain amplitudes of around 1% or less produces persistent slip bands (PSB) with a characteristic dislocation structure. Nearly all the applied plastic strain occurs within the bands. The bands have been studied most thoroughly in single crystals, but they also occur in polycrstals. PSBs are the usual precursors to cracking in ductile single-phase metals. In single crystals oriented for single slip, cracks can be formed at bands undergoing only primary glide and associated cross-slip: secondary slip is not necessary. Furthermore, there is a systematic mechanism leading to extrusions and very sharp associated cracks which come in from the surface and run along the interface between the band and the inert matrix in which it is embedded. Figure 2 is a composite picture of the process.

The structure of the PSBs is a periodic array of walls of edge dislocation dipoles, threaded by screw dislocations, not shown in Figure 2, which can run between the walls. The spacing of the walls is of the order of microns (10^{-4} cm), variable from metal to metal, and temperature dependent. Alternating plastic flow is accomplished by the backward-and-forward movement of the screw dislocations. The maximum alternating shear stress which can be borne by the structure is that which can just separate a bowing screw dislocation from a neighbour of opposite sign, and the maximum plastic strain amplitude is that which can be accomplished by the movement of the screws before they mutually annihilate one another by cross-slip. This maximum shear stress is identified with the fatigue limit of the single crystal, and suitably resolved with that for a polycrystalline array. The magnitude of the wall spacing controls the stress level, and is in turn controlled by the distance apart of two screw dislocations of opposite sign,

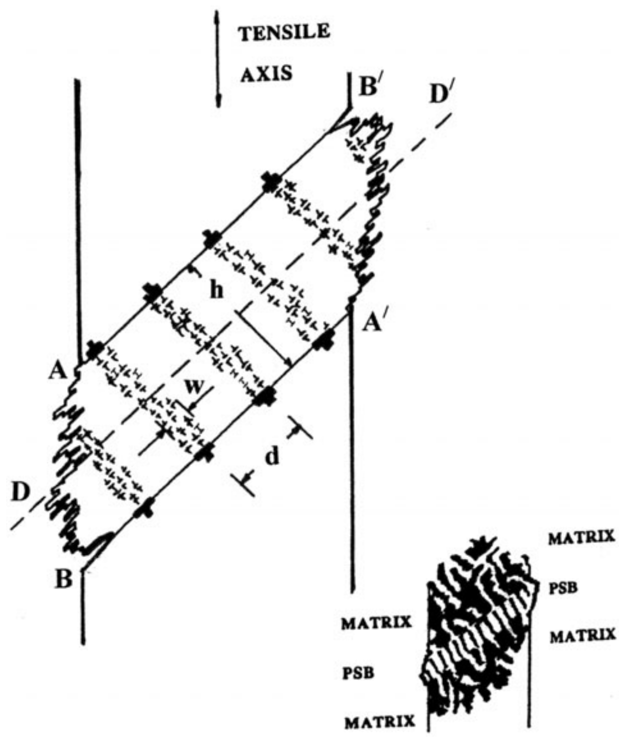

Figure 2. Schematic drawing of a PSB with dislocation structure and cracks at points B and B′. An impression of the PSB embedded in the inert matrix is shown lower right. The distance scale, determined by cross-slip, is set by the wall spacing d, which is about 1.3 μm in copper at room temperature; this also sets the minimum width h of the PSB. The walls are of width $w \approx 0.2$ μm, nearly independent of temperature, unlike d. Each wall supports about one dislocation of random sign on each crystallographic slip plane, each dislocation closely partnered by its opposite: a consequence of dipole refinement [18]. The bias towards vacancy dipoles results at each wall end in an effective virtual dislocation of Burgers vector b. The virtual dislocations are shown black and heavy and the tensile fibre strain along DD is about equal to b/d. In the absence of diffusion, the volume of the extrusion is equal to the vacancy excess in the dipole distribution.

just on the point of annihilation. The fatigue limit thus appears to be a *plastic property* of the crystal structure, related only to the ease of cross-slip, and not to the presence of prior cracks. Because the fatigue limit is controlled by cross-slip, it is closely related to the onset of stage III hardening and the ultimate tensile stress. The fatigue limit and the ultimate tensile stress depend in the same way upon temperature and stacking fault energy. The ratio of the fatigue limit to the ultimate tensile stress is about one third.

The definition of fatigue limit used here relates to the appearance or not of PSBs in a single crystal. It applies primarily to face-centred cubic ductile metals. Experimentally, it is to within a few percent equal to the endurance limit at 10^7 cycles, as listed in engineering data.

The above description summarises much beautiful work. Recognition of the crucial role played by PSBs, and the coining of the term itself is due to Thompson, Wadsworth and Louat [19]. Special mention must be made of Winter [20], who greatly clarified the three-dimensional structure of persistent slip, and of Mughrabi's [21] studies of that structure with the screw dislocations anchored by neutron irradiation in the process of movement. Papers by Brown [22,23] analyse the dislocation plasticity; reference to other analyses can be found in these papers.

The unanswered question, posed by Cottrell in the quotation above, is: how does this relate to the initiation of cracks? An answer lies in the fact that the dislocation dipoles which form the PSBs show a majority of vacancy type (half-planes pointing outwards) as opposed to interstitial type (half-planes pointing inwards). Such an array of dipoles produces tension parallel to the primary Burgers vector in the band, as if it were a plate or fibre in a stretched composite. The fibre stress produces no force on the primary dislocations, so it does not affect the glide properties of the PSBs. But where the bands meet the free surface, just at the boundary of the band, the fibre stress produces a logarithmic infinity in the self-balanced surface stress, both a compressive stress and a tensile stress which can operate to open up a surface crack. Although it is possible that such a stress directly breaks the bonds of atoms at the surface, it seems much more likely that it enhances the absorption of vacancy dipoles there, and progressively produces a very narrow crack. When the crack has propagated sufficiently far, further than the width of the PSB, the energy-release rate associated with the fibre stress falls to zero, and the crack becomes dormant. Because the width of the bands is normally of the same order-of-magnitude as the wall spacing, dormancy settles in when the crack is several microns long.

This picture explains in principle the paradox of short crack growth and the initiation of cracks from smooth surfaces. It also accounts for the remarkable phenomenon of dormancy.

We turn now to a brief discussion of the forces behind the crack-forming mechanism.

3. Non-linear mechanics of crack and extrusion formation

There are two possible reasons for the preference of vacancy dipoles over interstitial ones.

The first reason relies on the fact that interatomic forces resist compression more than tension, so the energy per unit length of a vacancy dipole is slightly less than that of an interstitial dipole [24,25]. It follows that the stress required to split vacancy dipoles is slightly larger than for interstitial ones, and that where the dipoles are connected by screw dislocations, glide can substitute one for another. No diffusion is required for this process. Normally, the applied stress swamps the very small effective stresses resulting from the energy imbalance. However, when the applied stress is removed, adjustments can occur in the dipole structures, and over many cycles a bias is produced. It is estimated that the stress must be less than about 10% of the fatigue limit for the non-linear effects to predominate. In a push-pull test of zero mean stress, about 20% of the time is spent with less applied stress than this.

The second reason relates to the core structure of the dislocations. Again non-linear atomic forces play a crucial role. If intrinsic stacking fault is preferred to extrinsic fault, either because of dislocation core structure, or because of the interatomic forces which determine the fault energy, then the very fine faulted dipoles will be predominantly of vacancy type [26]. This reason has its origin in crystallographic structure. It is probable that both non-linear elasticity and crystallography play a role.

From an experimental point of view, there is now little doubt that the edge dislocation dipoles produced by either cyclic plasticity or monotonic plasticity show a majority of vacancy type. Antonopoulos, Brown and Winter [27] found in copper cycled at room temperature that essentially all of the faulted dipoles contained intrinsic stacking fault, that is, were of vacancy type. Furthermore of 38 perfect (non-faulted) dipoles whose signs could be determined, 26 were of vacancy type. In nickel cycled at 600 and 750 K, Tippelt, Bretschneider, and Hähner [28] found that the faulted dipoles were all intrinsic, and of 91 perfect dipoles, 53 were of vacancy type. The bias to vacancies seems unaffected by the cycling temperature. Putting these results together, the bias to vacancies is approximately 2.5 standard deviations from the mean, a 2% chance if the distributions were random. In monotonic deformation, recent weak-beam studies by Niewczas [29] of copper show a high density of primary edge dislocation dipoles, predominantly of vacancy type, chopped into loops of 10–20 nm dimension. Although these experiments are tricky, it is evident that dislocation plasticity tends to produce an array of dislocation dipoles biased towards vacancy type. The bias is much more pronounced for faulted dipoles. Dipole faulting in face-centred cubic materials occurs with no net change in the vacancy content of the dislocation array.

A significant counter example is the observation by Lagerlöf, Castaing and Heuer [30] of interstitial faulted dipoles in α-Al_2O_3 (sapphire) deformed at high temperature. This relates to the mechanism for converting perfect dipoles to faulted ones, attributed by the authors to a point defect mechanism for the conversion process.

Whatever the reason for the imbalance, if glide processes can produce it, they will maintain a fibre stress. The energy of the PSB is reduced by the ejection of interstitial dipoles to the surface, leaving vacancy dipoles behind. But the resulting fibre stress incurs an energy penalty. If one thinks of the fibre strain, proportional to the fibre stress in the band, it is simply proportional to the imbalance between the types of dipole. As interstitial dipoles are replaced by vacancy ones, dislocation line energy is reduced linearly in proportion to the fibre strain. But the resulting overall elastic energy is increased proportionally to the square of the fibre strain. Thus, there is an equilibrium fibre strain and stress.

The equilibrium is maintained mechanically. No thermally activated process is required, not even cross-slip. Alternating external plastic strain or stress is necessary, but nothing else. Estimates of the fibre stress based on this mechanism produce order-of-magnitude agreement with the rather uncertain experimental estimates.

The fibre strain is very small. It must produce a stress smaller than that which would activate secondary slip, which hardens the PSB and renders it inactive. In effect, the fibre strain must be less than the Burgers vector divided by the wall spacing, about 10^{-4}. With a millimetre grain size, where PSBs meet the surface, the unrelaxed fibre strain produces a bump or extrusion about 0.1 μm high. Such extrusions are proportional in height to the grain size or to the width of the single crystal. This is in keeping with observations at low temperatures where diffusion can play no role. However, at higher temperatures, the extrusions will steadily grow to maintain the equilibrium fibre strain.

Figure 3 shows in more detail how the mechanism operates. At low temperatures, diffusion is not possible. Screw dislocations (not shown) move in and out of the page,

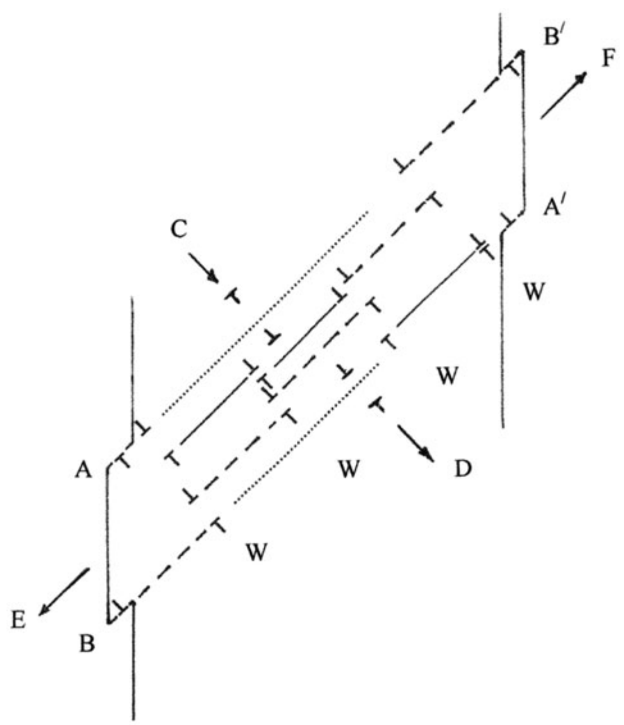

Figure 3. Schematic staircase slip [25,31] showing how unlimited extrusion growth can occur when short circuit diffusion is possible. (An error in labelling in [25] has been corrected.) When the PSB is unloaded, dipole exchange [24] occurs within the walls (labelled W) to eject larger interstitial dipoles and retain smaller vacancy ones. The resulting tensile fibre stress attracts more interstitial loops from the matrix, and repels vacancy loops. Dipoles and loops which straddle the interface are subject to these forces. The loops move by conservative climb as shown at C and D. The resulting departure from the equilibrium fibre strain is corrected by expelling interstitial loops by glide into the extrusions at E and F. Further climb of loops in the resulting loop density gradient near the PSB allows the extrusions to grow without limit, draining material from the entire matrix.

cross-slipping to annihilation and depositing edge dislocations in the form of dipoles. Between extremes of tension and compression, in the absence of external load, in the interior of the crystal, non-linear forces operate to produce narrower, but more numerous, vacancy dipoles and wider, less numerous, interstitial dipoles. The latter are split and glide to the surface where they become extrusions. This produces 'staircase' glide, as depicted in the diagram by Essmann, Gösele and Mughrabi [31]. The difference is that Essmann et al. postulate the disappearance of the stress field of the smaller vacancy dipoles, leaving the PSB in compression, rather than in tension, as proposed here. If the band is in tension, at temperatures high enough to allow pipe diffusion to confer climb mobility to dislocation loops and dipoles, interstitial loops with a primary Burgers vector will be drawn by elastic forces into the PSB, and vacancy loops repelled.

The excess interstitial loops will be ejected to the surface by the alternating plastic strain in order to maintain the equilibrium fibre stress. A concentration gradient of loops will be set up near the interface between the band and the matrix, and by diffusion of the loops in the gradient, almost unlimited growth of the extrusions can occur. The non-linear force which distinguishes interstitial from vacancy dipoles acts as a ghost in the machine to produce the extraordinary extrusions from alternating shear.

The question arises: above what temperature can thermally activated diffusion of loops occur? The literature seems not to offer a clear picture. A simple view to take is that the activation energy for pipe diffusion in the core of a dislocation is roughly that for divacancy motion. It is thought that these diffusion processes become operative above about one-quarter of the melting point, but it is difficult to give a precise answer to the question.

4. Energetics of stage I cracks

It seems very difficult to model the forces on the cracks from initiation to dormancy. Brown and Ogin [32] show that if the fibre stress is tensile, then at the intersection of a PSB with the smooth surface there is a line of formally infinite tension where the corner of the matrix makes an obtuse angle, points B and B', Figure 2, and infinite compression where the corner of the matrix makes an acute angle, points A and A'. Physically, one can imagine the tension of the fibre stress with a component at the surface pulling the surface apart at B, but pushing it together at A. It does not matter how small the fibre stresses are, because the tractions acting along the whole band must be compensated at the surface, so the stresses there still approach infinity as the length of the band. Although cracks are most commonly seen at B sites, there are many observations of crack initiation at A sites, and many sites where both are seen at the same time. The cracks always run along the interface between the PSB and the matrix, which means that they do not result from random slip processes within the band. There are two complications which prevent simplicity: firstly, in many cases the PSB makes a small angle with the primary slip direction, and thereby generates a fibre stress which alternates in sign with the shear; and secondly, when the band is first formed, it is likely to be accompanied by a reduction in overall dipole density, and therefore to be in compression until the equilibrium fibre stress is achieved. The first cracks or intrusions are therefore expected at side A, to be followed by more dangerous cracking at side B as the cycling continues. This pattern seems consistent with the most recent results: see the excellent comprehensive papers by Man et al. [33,34]. The 'infinite' stresses at the critical corners are a product of the continuum approximation for the dislocation distribution, and therefore are a mathematical artefact. However, at the cores of the 'real' dislocations there are more serious singularities: broken bonds which can initiate cracks under the very large tensile stresses due to collective effects. A vacancy dipole near the points of infinite stress will be subject to a very large force drawing it to the surface, thereby initiating a crack. On such a view, the cracks will initiate at the same time as the PSBs form, in general agreement with observation. The reader is strongly recommended to look again at Forsyth's early paper [9] where there is a diagram showing the action of tension at point B and perhaps even compression at point A.

It is much easier to deal with the crack when it has progressed further than the width of the PSB. Brown and Ogin [32] present a simple formula due to J. D. Eshelby showing that the energy release rate for such a crack diminishes inversely proportional to the length of the crack: the crack becomes dormant. When it is shorter than the Griffith length, it can grow only by accretion of vacancy dipoles, with no other driving force. An estimate for the dormant length is given: it is about ten times the width of the PSB. Wide bands are more dangerous than narrow ones, because the dormant cracks are longer and are closer to propagation as stage II (subcritical) fatigue cracks. The dormant cracks will be very sharp because there is not enough stress intensity to drive plasticity at the tip.

During the early stages of the formation of surface relief, both cracks and extrusions will grow by the rate with which screw dislocations transfer edge dislocations from one dipole to another. This occurs about once per cycle according to Antonopoulos and Winter [35], so the growth rate is about one Burgers vector per cycle. A few hundred cycles establishes the equilibrium extrusion. After that, in the dormant state, at low temperatures, the crack will grow by about one Burgers vector per cycle, although the extrusion in equilibrium will not grow. The crack growth rate is then about one micron for every 3000 cycles – consistent with observations by Basinski and Basinski [36]. However, if short circuit diffusion around loops and dipoles enables interstitial loops to enter the PSB, and vacancy loops to be ejected from it, the extrusion will grow indefinitely at a rate limited by the slower of the plastic process and the thermally activated diffusion processes.

Because of this linear slow growth, any condition on the transition from stage 1 crack growth to subcritical stage 2 growth and fracture will be linearly dependent on the number of cycles. Brown and Ogin [32] propose a very crude model, which suggests that failure occurs at a fixed cumulative strain of about 600. Although the model deserves improvement, it is not inconsistent with the rather sparse data. What is important is that it predicts failure at many fewer cycles than the Coffin-Manson law, which cannot apply for high cycle fatigue with its unique dislocation mechanism for crack initiation. The way forward seems to be through more systematic observation using modern techniques, as pioneered by Man et al. [34].

At higher temperatures, where the extrusions can steadily grow, the model proposed here is closely related to that of Polák [37], in which individual vacancies produced by dipole annihilation within the PSBs diffuse outwards. The vacant sites cause intrusions, while the atoms they leave behind end up in extrusions. The resulting surface profile is symmetrical, an extrusion sandwiched by intrusions. Polak's model requires individual vacancy mobility, as well as vacancy formation at the dipole debris. The model proposed here requires dislocation glide, core diffusion, and the elimination of screw dislocation dipoles by cross-slip. Both Polák's model, and that of Essmann, Gösele and Mughrabi, visualise a compressive fibre stress, whereas the fibre stress resulting from the energy difference between vacancy and interstitial dipoles should be tensile. It leads to extrusions and cracks resulting from glide processes only. It can occur at the absolute zero of temperature.

5. Can crack initiation be inhibited by alloy design?

Shot-peening is traditionally used to prevent or delay surface cracking by fatigue. It produces compressive surface stresses which counteract the dangerous tensile surface stress produced by PSBs or indeed by any other cause. It is very effective, but costly, deployed only on those moving parts which require it. Might there be another method based on the improved understanding of crack initiation by persistent slip?

Regardless of the type of chemical binding, the interatomic potential will act to resist compression more than tension, and so favour vacancy dipoles over interstitial ones. The Grüneisen constant, which is a dimensionless measure of the effect, is about equal to two for a wide range of materials. It is proportional to the thermal expansivity. One might think of alloys based on invar, where zero thermal expansivity is achieved by balancing normal expansion against contraction due to phase transformation. However, the dipoles which must be controlled to inhibit cracking are of nanometre size, so that any control must operate at a near-atomic level, whereas the phase transformations are on a much larger scale. A possible clue is offered by the observation of interstitial faulted dipole formation in sapphire [30]. This suggests that one should think of alloying to control dislocation cores to promote extrinsic faulting, thereby nullifying the pervasive non-linear elastic forces. Such a possibility is intriguing but seems remote. Extrinsic faulting has been observed: see Hirth and Lothe [26].

6. Conclusions

The fundamental puzzle posed by Cottrell [17] seems to be solved. One can understand how a crack which is energetically impossible – that is, of less than the Griffith length, and therefore non-propagating even in an ideally brittle solid – can be initiated because of internal stress resulting from non-linear forces acting in conjunction with plastic flow. One can further understand how such a crack grows ever more slowly until it becomes dormant or nearly dormant at a characteristic length related to dislocation processes. One can also understand how extraordinary scrolls of extrusions grow as external extensions of PSBs subject to cyclic plasticity at moderate temperatures. It seems also possible perhaps to achieve metallurgical control over such processes.

Acknowledgements

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