

Strain Concentrations in Tensile, Fatigue and Fracture Behaviour

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Abstract A critical survey has been made of tensile, fracture, shear banding and fatigue measurements and interpretations reported for different types of materials and test conditions. The mechanical properties of the materials are shown to be largely determined by microscopic plastic strain concentrations which depend on the inhomogeneity of the material microstructure, especially including importantly inhomogeneity of the dislocation substructure. Understanding this inhomogeneity is shown to provide a number of connections between seemingly disparate phenomena. The evolution of the dislocation substructure and its relationship to crystallography and various levels of microstructure are critically important. Professor Cottrell made seminal contributions to understanding the fundamental mechanisms involved in determining such strain concentrations. His work continues to provide clarity and guidance to current research accomplishments.

Keywords Pile-ups, Cleavage, PLC, ASB, PSB

1. Introduction

An article entitled "Plastic Strain Localizations in Metals: Origins and Consequences" has just been completed for the 2013 publication of the periodical: Progress in Materials Science [1]. The article has provided the basis for us to report in the ICF13 Cottrell Memorial Symposium on a number of important sub-topics on which Alan Cottrell has paved the way forward to modern developments. Four such sub-topics are:

(1) The Cottrell virtual work equation for a single-ended dislocation pile-up was first reported in Progress in Metal Physics [2] preceding Cottrell's seminal book on dislocations [3]; the equation is

$$\tau^* = n\tau_o \quad (1)$$

Where τ^* = stress at blocking obstacle, n = total number of dislocations in pile-up, τ_o = effective applied stress.

(2) The Cottrell-Bilby carbon locking of dislocations theory which provided a basis for understanding the Portevin-Le Chatelier (PLC) effect of serrated plastic flow;

(3) The Cottrell dislocation crack reaction for understanding cleavage in bcc metals and related materials; and

(4) The Cottrell-Hull analysis of slip band intrusions/extrusions for fatigue crack development associated with persistent slip band structures.

2. Deformation Behaviour – Dislocation Pile-ups

One of the most important parameters in a vast array of materials is grain size and the effects of grains on deformation, a topic to which Prof. Cottrell has made numerous contributions. His work was followed by the well-known Eshelby, Frank and Nabarro (EFN) analysis for the $n - \tau_o$ relationship in the equilibrium equation for the pile-up dislocations spread over a length, L [4]:

$$\tau_o = \frac{Gnb}{2\pi kL} \quad (2)$$

In Eq. (2), G is shear modulus, b is dislocation Burgers vector, and $1 \geq k \geq (1 - \nu)$ for screw or edge dislocation character respectively with ν being Poisson's ratio. Substitution for n in Eq. (1) and taking $\tau_0 = \tau_{ys} - \tau_i$, leads to the Hall-Petch equation for yield stress, τ_{ys} :

$$\tau_{ys} = \left(\frac{Gb\tau^*}{2\pi k} \right)^{\frac{1}{2}} L^{-\frac{1}{2}} + \tau_i = \tau_i + k_y L^{-\frac{1}{2}} \quad (3)$$

In Eq. (3), τ_i is a “friction” stress and k_y is now known as the microstructural shear stress intensity. Taking the pile-up length, L , to be equal to the average polycrystal grain diameter, ℓ , then Eq. (3) can be written in terms of tensile stresses:

$$\sigma_{ys} = \sigma_o + k_y \ell^{-\frac{1}{2}} \quad (4)$$

One may view yielding as a process in which the local shear stress at the tip of a slip band builds up with each additional dislocation and eventually reaches a level at the boundary or nearby in the adjacent grain to trigger transmission of plastic deformation through the boundary. The microstructural stress intensity parameter, k_y , clearly controls this process and as such is, in principle, both temperature and strain rate dependent in addition to having sensitivity for other aspects of the materials microstructure.

The build-up to reach the critical stress is most rapid as the first few dislocations pile up against a boundary. The effect of adding one dislocation to the pile up, $\Delta n = 1$, in Cottrell's Eq. (1) gives:

$$\frac{\Delta\tau}{\tau} = -\frac{1}{n} \quad (5)$$

Thus, the fractional decrease in stress necessary to reach the threshold for spreading plasticity decreases with each additional dislocation added to the pile-up. In essence, this describes the reduction in Hall-Petch stress provided by increasing the slip length (by increasing the grain size), so as to facilitate overcoming an obstacle to plastic flow. The model result is illustrated in Fig. 1.

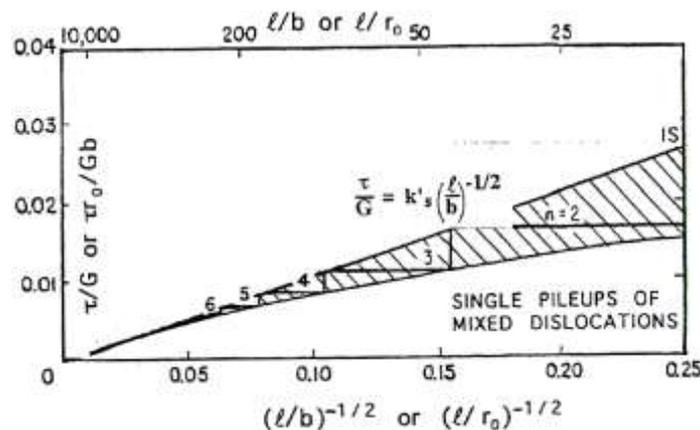


Figure 1. Normalized yield stress vs. reciprocal root of normalized grain size in metals. The core radius is r_o [5]. The integers represent the number of dislocations in the pile up.

Figure 1 also illustrates the lowered flow stress with an increased number of dislocations. It also illustrates the reason for “scatter” in the mechanical properties of ultra fine grained materials and nanocrystalline materials. Since slip bands cannot have fractional numbers of dislocations, a range

of grain size will contain, say, three dislocations. For two dislocations, say, to be in the pile-up the grain size must decrease to a pre-determined size. Joining the tips of the “steps” gives the envelope of possible values for the flow stress. Small grain sizes and low numbers of dislocations in them also relate to the improbability of cleavage in fine grained Fe as described by Armstrong and Antolovich [6] as discussed below.

3. Strain Concentration and Fracture

An updated model for plastically-induced cleavage fracturing of bcc and related metals and alloys is shown in Fig. 2. The basic model fracture had been developed originally by Cottrell [7].

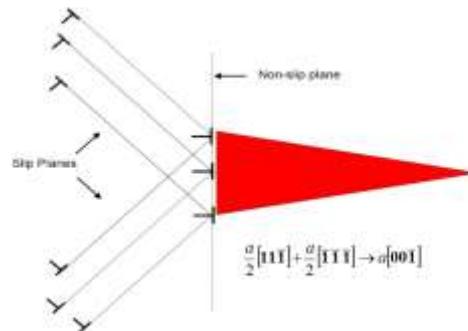


Figure 2. Cottrell model for fracture in BCC (α) Fe [7]

In this model, parallel dislocations on intersecting slip systems (i.e. $\{110\}$ -type planes) react to form a sessile dislocation on a non-slip $\{100\}$ plane thus providing a cleavage crack nucleus. Repetition of this reaction promotes growth of the microcrack until it is large enough to satisfy a Griffith-type criterion and spread by cleavage on a $\{100\}$ type plane. The reaction shown in Fig. 2 is vectorily correct and energetically favourable. Furthermore, careful observations showed that *fracture occurred only after some plastic deformation* as would be required by this model. The model has been applied to explaining crystallographic aspects of cleavage fracture in other crystalline structures, for example, at indentations on MgO (001) crystal surfaces [8]. However, not all reactions such as that shown in Fig. 2 actually result in good predictions of cleavage. Antolovich and Kip [9] pointed out that not only must the reaction be energetically favourable but one must also consider the force barrier to be overcome. An analogy would be two parallel dislocations on parallel planes. Their lowest energy position is when they are lined up vertically forming a finite segment of a low angle tilt boundary. However, to bring the dislocations into the position shown, a force barrier must be overcome which is a maximum when a line joining the two dislocations is inclined at 22.5° to the slip planes. Once aligned there is a restoring force directed against separation. Antolovich and Kip considered: (1) the effect of angular orientation of the two dislocations on the forces that must be overcome to form a crack nucleus and (2) the forces required to bring an additional dislocation to within a Burgers vector of the crack nucleus. The problem that they considered is illustrated in Fig. 3. The results were illuminating. First of all, with respect to BCC structures and α -Fe in particular, the calculations showed that for almost all angular orientations as defined above, glide dislocations are attracted to a common junction implying that overcoming the Peierls force would be sufficient to form a crack nucleus. This was in opposition to most other crystal structures (e.g. intermetallics, FCC crystals) in which such attractive ranges were rare. However, once formed, it becomes increasingly difficult to grow the crack since the back stress due to the nucleus requires additional force to move a dislocation into the vicinity of the nucleus (i.e. to grow the incipient crack). Based on these detailed calculations, one would expect

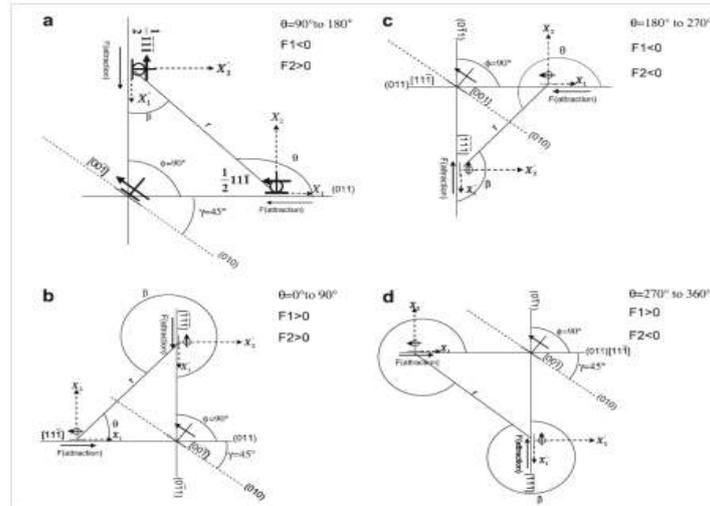


Figure 3. Two parallel reacting dislocations in BCC crystal structure. The axis system for each dislocation as well as angular variables are defined in (a). The signs of the forces on dislocations 1 and 2 that cause attraction to a common junction are shown in (a–d) for all possible angular orientations.

cleavage to be prevalent at low temperatures, which is observed in α -Fe, and some plasticity to precede cleavage, which is also observed.

The pile-up model is currently being used in to study near theoretical limiting stress levels reached for nanopolycrystals on a Hall-Petch basis. Antolovich and Armstrong considered possible modification of the Hall-Petch effect for cleavage of α -Fe if only a small number of dislocations were involved [6]. They computed the dimensional scale at which a stress concentration from the pile-up could duplicate that of a cleavage crack. As shown above, the pile-up approach can be applied at rather small dimensions and can also be used to explain “scatter” of strength data. Importantly they showed that for small numbers of dislocations the slip band generated stress computed directly for small numbers of dislocations can never reach the crack-like stress (computed using continuous distributions of dislocations) implying that at small grain sizes (and small numbers of dislocations) cleavage is improbable. The results of their calculations are shown in Fig. 4.

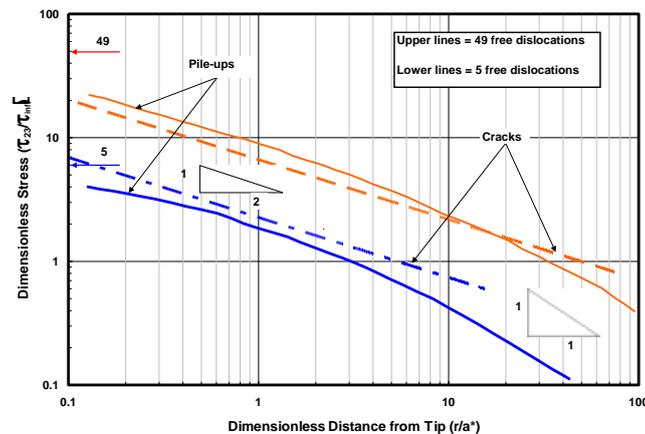


Figure 4. Dimensionless shear stress vs. dimensionless distance from crack or slip band tip (normalized to the crack length) [6]. For five free dislocations, the stress ahead of the slip band falls below that of a crack and cleavage is unlikely. Note further the crack like behaviour near the tip of the slip band (slope of $-1/2$) and the traditional slip band like behaviour (slope -1) for multiple Burgers vector representation.

The same result was obtained on incorporation of Griffith crack tip modification as prescribed with gradient elasticity theory (GET). Another related application of such pile-up model consideration, to be developed in Section 5, is to evaluate the breakthrough of a pile-up in providing a fundamental explanation of adiabatic shear banding behavior. In such case, the rapid avalanche-like dissipation of the stored energy in pile-up provides a ready energy source for appreciable thermal heating [1].

4. Strain Concentration in the Portevin-Le Chatelier Effect

The French researchers, A. Portevin and F. Le Chatelier discovered that for certain combinations of strain rates and temperatures the stress-strain curves of Al-Cu-Mn and Al-Cu-Mn-Mg alloys exhibited serrations in the stress strain curves and that fairly well-defined bands formed in the gage length of the specimens [10]. This discovery, now eponymously known as the PLC effect, has been of keen interest in the 90 years since it was first observed and to this day controversy exists in terms of the basic mechanisms and the effect on mechanical properties such as fatigue. It was not until the advent of dislocation theory that the outline of an understanding was developed and again Prof. Cottrell played a key role in clarifying, after his work with Bilby [11], the underlying physics of the process [12]. The model that evolved was based on the concept of thermal activation. For certain régimes of strain rate and temperature there is a dynamic interaction between solute atoms (e.g. C in Fe-C alloys, Mg in Al-Mg alloys) and dislocations such that there is a repeated locking and escape mechanism attributed to the mobile dislocation density.

During locking, the stress climbs for the dislocations held back by their “atmospheres” and when the dislocations escape, the stress drops. The process is repeated throughout the test. Thermal activation energies have been measured for this mechanism by numerous investigators and while one may object to some of the approaches used, it is clear that activation energies are on the order of that of diffusion of the solvent species [13,14]. Recent data for IN100, a Ni-base superalloy strengthened by the coherent $L1_2$ precipitate γ' is shown in Fig. 5 [15]. In Fig. 5 the temperature strain rate plane is divided into regions in which the PLC effect is observed and not observed. The boundary between the two regions marks the onset of the PLC effect and as such may be used to determine the activation energy which is 1.14 eV and comparing reasonably well to the activation energy for bulk diffusion of C in Ni of about 1.48 eV. However, there is an apparent contradiction in using the activation energy of an atom/dislocation pair and the large strains that are associated with the serrations and the corresponding large numbers of dislocations needed to carry that strain. In effect, currently-accepted theories describing this process appear to be incomplete. In broad outline, the deformation process is initiated by unpinning of the dislocations having the lowest effective unpinning stress. At this point, the free dislocation would encounter a more strongly pinned dislocation at a larger precipitate. However, the stress on the second dislocation would be essentially doubled since there would be a two dislocation pileup and the stress would drop. The group of two dislocations would next encounter a locked dislocation but the stress at the leading dislocation would now be three times the applied stress so, depending on the actual locking stress, the required stress to continue deformation would decrease. The process of increasing strain with decreasing stress would continue until all of the dislocations on a slip plane have been mobilized¹ [1]. We thus have a picture of a decreasing stress with increasing strain for the first slip plane. The next easiest dislocation to unlock would be activated elsewhere in the crystal and as it moves across

¹ This explanation is simplified and does not take into account the statistical distribution of the pinning points. This more realistic situation may be addressed through a detailed statistical analysis.

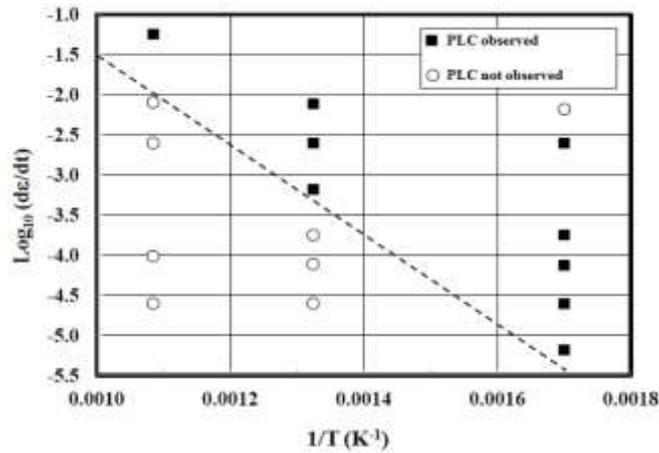


Figure 5. Arrhenius plot of deformation behaviour of IN 100 showing the boundary between PLC behaviour and non-PLC behaviour which gives an activation energy of 1.14 eV [5].

its slip plane the same process would operate. However, based on this model, the second slip plane to activate would do so at a higher stress because of the higher unlocking stress and the back stress due to the piled up dislocations in the first slip plane. Similarly the next source to operate would follow the same process but at an increased stress. Such a model would account for an accompanying Hall-Petch dependence that is known to apply for PLC behaviour. The pile-up mechanism implicitly accounts for ending the behaviour when all of the locked dislocations having relatively low unlocking stresses have been mobilized after which point deformation continues by normal flow processes. Thus this model description appears to account for:

- Temperature and strain rate effects through the initial unlocking of the initial dislocations on each slip plane.
- Macroscopic strain localization through local stress intensification at locked dislocations by the mobile dislocations.
- Exhaustion of the phenomenon through strain hardening due to the distribution of unlocking stresses, and activating normal flow processes at some stress level.
- An increasing mean stress (cyclically increasing flow stress) due to interactions from piled up dislocations and a generally increasing for each slip plane.

Extension of the Cottrell-Bilby model to the PLC effect has an interesting connection to the modern thermally activated strain rate analysis (TASRA) for dislocation plasticity. A positive or negative strain rate sensitivity (SRS) may occur according to whether one is on the upside or downside of the added PLC thermal activation curve [1]. Given that the PLC process is thermally activated, the following functional dependence is implied:

$$\tau_{th} = f(T, \ln \dot{\gamma}) \quad (6)$$

Here the symbols on the right have their usual meaning. However, some attention must be paid to the meaning of τ_{th} which is that component of the flow stress above long range internal stresses. There are examples in the literature in which it is mistakenly taken as the total stress which results in some errors in activation energies and over-all understanding. From calculus, Eq. (6) may be used to give the result:

$$\left(\frac{\partial \tau_{th}}{\partial T} \right)_{\ln \dot{\gamma}} \cdot \left(\frac{\partial T}{\partial \ln \dot{\gamma}} \right)_{\tau_{th}} \cdot \left(\frac{\partial \ln \dot{\gamma}}{\partial \tau_{th}} \right)_T = -1 \quad (7)$$

Equation (7) may be employed to provide insight into the PLC effect in terms of the separated factor dependencies. For normal dislocation velocity description with thermally activated shear stress, τ_{th} , the first factor in Eq. (7), is negative and the second two factors are positive. The same equation is usefully applied to the analysis of the incremental PLC effect for τ_{th} . Note that when the third term is negative (as seen for PLC), then each of the first two terms *must* be positive. Thus a negative strain rate sensitivity of the flow stress for dynamic strain aging (PLC) is associated *only* with the stress rising to the peak of strain aging and not for an “over the top” régime of decreasing stress. Misunderstanding of this feature has led to some controversy in the literature about the analysis of the PLC activation energy.

5. Strain Concentration and Adiabatic Shear Banding

Adiabatic shear banding refers in a formal sense to the case in which a localized shear band forms with no transfer of heat to or from the external environment (i.e. $\delta Q = 0$). The behaviour is favored in metals under conditions of low heat capacity and low thermal conductivity when deformed at high loading rates and/or low temperatures. The mechanical work associated with formation of the shear band is mainly transformed into heat and thereby manifested by an increase in temperature. *Unlike the PLC effect which is self-exhausting, the formation of adiabatic shear bands (ASBs) is self-amplifying and leads to localized failure.* Recall that adiabatic shear banding was first observed by Tresca in a set of forging experiments on a Pt-Ir alloy [16]. When hammered just below the “red-hot” temperature, distinct X-type shear lines appeared on the longitudinal cross-section of the test specimen indicative of an exceptional temperature increase.

Eshelby and Pratt [17] used the mathematical solution for the temperature increase associated with a moving source of energy provided by Carslaw and Jaeger [18] and modified it to rows of equally spaced dislocations passing by a fixed lattice point. The main result of their calculation was:

$$\Delta T = \tau_o(nb)v/2\pi K \left(\frac{\pi\Lambda}{2L}\right)^{\frac{1}{2}}, \Lambda \ll L \quad (8)$$

Where v is the dislocation velocity, K is the thermal conductivity, L is the length of the slip band and Λ is an effective thermal a length given by:

$$\Lambda = 2\alpha/v \quad (9)$$

where α is the thermal diffusivity. Using reasonable values for Al, they showed that on the basis of this model, temperature increases of only 2° K was obtained from the model calculation. Furthermore, they examined other arrangements and concluded that no arrangement could be found which would give a large temperature increase. However, the very earliest work of Tresca proved that high temperature increases were occurring and thus the model of Eshelby and Pratt is a very useful step in developing a more complete understanding. This issue was re-examined by Coffey and Armstrong [19] on the basis of further accumulated evidence that appreciable temperature rises were being evidenced in shear banding experiments, A model favorable to shear banding was envisioned of isothermal stress build-up of stored energy in a dislocation pile-up, then leading to sudden obstacle collapse, and rapid dissipation of the stored energy by very localized plastic work in an earthquake-like dislocation avalanche. The model led, with employment of well-established slip band mechanics [20-21], to an expression for ΔT given by:

$$\Delta T < \frac{k_s L^2 v(1-\nu)}{10\pi^2 K(1-2\nu)} \ln\left(\frac{2K}{c^* v \Delta x_i}\right) \quad (10)$$

Where L is the grain size, k_s is the Hall-Petch microstructural stress intensity parameter, c^* is the specific heat at constant volume, ν is Poisson's ratio, Δx_i is the spacing of dislocations in pile-up and v is the terminal dislocation velocity. Using an upper limit for the dislocation velocity of the shear wave speed and with other parameters for steel, a value of $\Delta T < 3.2 \times 10^3$ K was obtained. The over-estimated temperature rise for pile-up collapse was taken to give credence to the mechanism. Experimental results obtained on shear plugging of Ti-6Al-4V alloy material produced regions of sprayed molten metal onto the shear plug walls, consistent with prediction of the pile-up avalanche mechanism.

6. Strain Concentration in Fatigue-Persistent Slip Bands

It has long been known that fatigue loading results in roughening of the surface and that the bands in which deformation is carried are of a "persistent" nature [22]. Persistent slip bands (PSBs) have long been a subject intense research but it was not until the development of dislocation theory that some understanding of the fatigue process could be established on a physical basis. This too was a field in which Prof. Cottrell provided initial insight [23], particularly on the formation of slip band intrusions and extrusions. Considerable research has been carried to understand the details of this important phenomenon and a broad outline has emerged in which a unique structure is developed, at least in FCC single phase materials, of which Cu has received by far the most attention. A representative PSB is shown in Fig. 6. It consists of dislocation walls of primary edge character bounded by edge dislocations on the top and bottom surfaces with cyclic deformation being carried by screw dislocations. Controversy exists as to the signs of the dislocations at PSB boundary, the

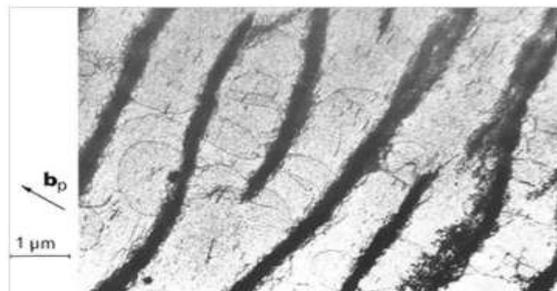


Figure 6. Walls in persistent slip bands (dark regions) and gliding screw segments in the channels between walls [24].

state-of-stress within the PSB's [25], the nature of intrusions, and the mechanism of crack formation [27]. Complex processes take place on the PSB walls which result in excess vacancy production. Evidence of this is found in the fact that a single PSB produced extrusions on both sides of a single crystal of Cu and also in the fact that at high temperatures the vacancies can migrate to sinks and the PSB's are actually thinner than at low temperature [28]. These ideas have been used with some success to numerically model crack nucleation at grain boundaries in Ni-base superalloys by accounting for the system energy including importantly the energy in the PSB and taking crack nucleation at an energy extremum. Of course application of the PSB morphology to precipitate systems may require some modification. An actual PSB taken from a fatigued René 95 LCF specimen is shown in Fig. 7 [30]. The morphology is very different from that shown in Fig. 6.

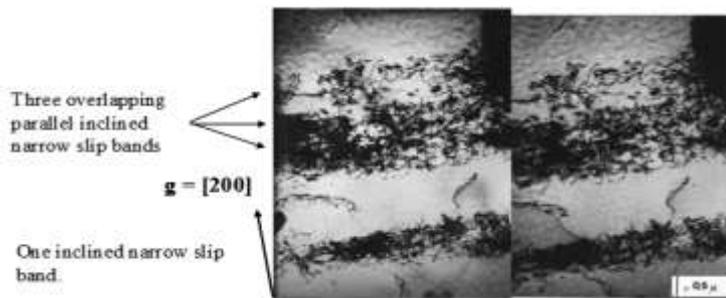


Figure 7. TEM Stereo pair of dislocations in fatigued René 95 [30] showing that there are four narrow slip bands, three of which are overlapping. Such information can serve to develop physically accurate models.

7. Summary

In this paper connecting the pioneering researches of Alan Cottrell and a current review of modern research results, we have demonstrated a critical role for localized strain concentrations in several deformation, fracture and fatigue processes. In all cases, the strain concentration arises from inhomogeneities in the microstructure including the dislocation substructure. The subject is not complete in that our understanding remains lacking in many important areas such as for PSB's in precipitate-bearing alloys. Accurate assessment of the true precipitate and dislocation structure will provide a sound basis for numerical modelling of industrially important materials and should also improve our ability to develop fatigue-resistant structures. In most of the literature, the effects of slip mode have been largely ignored and studies in which slip mode is varied (e.g. by controlling stacking fault energy) would be of great value.

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