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"A Combined Macroscopic and Microscopic Approach to the Fracture of Metals"

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Abstract

The work accomplished during the contract period July 1976 - June 1977 includes the completion of a comprehensive study of the contributions of dislocation substructures and local stresses at particle interfaces to the strain hardening of dispersion hardened steels, and the presentation of a model of segregant induced embrittlement of grain interfaces. Also, work was continued on crack initiation at inclusions and on the theory of plastic flow localization. These microscopic effects are discussed in relation to the mechanisms of brittle fracture and ductile rupture of metals and alloys.

On a more macroscopic scale, the state of stress and strain associated with the large plastic deformation at a crack tip was further defined based on finite element and slip line calculations, and some preliminary results have been obtained by finite element methods for stable crack growth under plane strain conditions. Also, a new finite element method has been developed for fully plastic flow under plane strain conditions.

A major effort has begun on an experimental study of environmental effects on interfacial separation, specifically the hydrogen assisted fracture of medium and high strength steels.

CONTENTS

A. Detailed Description of Research Program

1. Role of Particles and Interfaces in Strength and Fracture

a. Particle and Sub-Boundary Strengthening in Steels

As we discussed in our last progress report, an important aspect of our comprehensive program on the deformation and fracture of carbon steels, and in particular of spheroidized plain carbon steels, has been a thorough study of their strain hardening behavior. Our viewpoint has been that there are varied contributions to the overall hardening which arise from interactions in the grain matrices between dislocations and particles, between dislocations and sub-grain boundaries, and between dislocations and grain boundaries. One main objective of this study, which was begun by Gurland and Anand and continued by Asaro, Chang, and Gurland has been a determination of these individual contributions especially as they are concerned with the details of the particle-matrix interfacial stress state. With the recently completed work of Chang (Thesis and Technical Report COO-3084-51; also the publication by Chang and Asaro) we have essentially met this objective. For example, we have now developed a strain hardening law for these steels which superposes all these hardening contributions and yields workhardening curves which accurately describe our latest experimental results for two steels with carbon contents of 1.4 and 0.8 percent by weight. The effects on strain hardening of varying particle volume fraction e.g. by using different compositions, and of varying particle size at a fixed volume fraction, by performing appropriate heat treatments, have both been studied experimentally. These effects have been accounted for, theoretically, in our dislocation models. In addition the role of subgrain boundaries was studied by preparing microstructures with and without subgrains. For the subgrains we note that while the subgrains generally increased the flow stress, they contributed little to the overall strain hardening.

An important contribution to strain hardening, which has direct relevance to the initiation of ductile fracture in these steels, is the development of long-range residual stresses which are caused by the incompatible plastic strains between the elastic particles and the plastic matrix. These stresses give rise to enhanced Bauschinger effects and to intense local stresses that act on the particle-matrix interfaces. Since these interfacial stresses are a prime contributor to interfacial separation (i.e. void initiation) we have made careful and extensive studies of the Bauschinger effects through cyclic loading and have used the analysis of Brown and co-workers (Phil. Mag. 1971-1976) and of Asaro (Acta. Met. 1975) to relate the measurements to the magnitudes of these stresses. Our findings indicate that the local stresses increase less than linearly with imposed plastic strain and generally lead to tensile stresses on the interfaces which reach saturation levels that approach one half the value of the flow stress. In the matrix there are "back stresses" which contribute a term to the strain hardening that can be expressed as

$$\sigma^{i} \approx 3\delta\alpha\mu f(\varepsilon_p^{0.3}/r^{0.7})$$

δ and α are well defined constants involving ratios of elastic constants, f is the particle volume fraction, and the exponent of 0.3 (rather than unity) on the plastic strain reflects the fact that most of the incompatible plastic strains are accomodated (or actually relaxed) through "secondary slip" which produces no long-range stresses. The effect of particle size can be accounted for by the term involving the particle radius, r. The above relation has been experimentally verified and is explained by our micro-plastic models involving dislocation-particle interactions.

We have also found that the concept of incompatible plastic strains or "unrelaxed strains" can be used to explain the transition in strain hardening behavior in these steels which is observed to set in at monotonic axial strains of about 0.04. At strains less that 0.04, the maximum normal stresses on the particle boundaries increase in proportion to ε_p^u where ε_p^u is found to be related to the plastic strain ε_p as

$$\varepsilon_p^u \propto \varepsilon_p^{0.3}$$

At strain levels approaching 0.04, ε_p^u and the back stresses appear to abruptly saturate, thus leading to a lower rate of strain hardening. This, according to our Bauschinger effect measurements, happens at the same strain values where the so-called "double-n" transition occurs and this correspondence provides an attractive micro-mechanical explanation for the effect.

The present work has contributed directly to our understanding of strain hardening in dispersion hardened steels and, since it was focused on providing a firm understanding of the dislocation substructures and local stresses at the particle interfaces, it has also directly contributed to our ongoing study of particle cracking and particle-matrix separation.

(Staff: R. Asaro, Y.W. Chang, and J. Gurland)

b. Void Initiation at Cementite Particles in Spheroidized Steels

The current experimental work deals with fracture at cementite particles in steels. Observations in uniaxially loaded steels (0.13 - 1.05%C) have revealed three main modes of void nucleation at particles, namely 1) transparticle cracking, with shape and/or internal boundary effects, 2) cavitation of matrix ligaments between near-neighbor particles, including matrix grain boundary effects, and 3) particle-matrix decohesion, with matrix boundary effects. The three fracture modes are listed in the order of frequency observed in uniformly deformed cross-sections. It has become obvious that the fracture initiation process at particles is very complex and is considerably influenced by the local microstructure of particles and matrix, in particular by the grain boundaries and sub-grain boundaries in particles and matrix. Pronounced particle size and concentration effects have also been noted.

The objective of this aspect of the work is to determine the condition of void initiation in the various modes as function of stress and strain, and particle characteristics and spacing. The theoretical analysis in progress is concerned with the calculation of the local stress intensities at the particle boundaries as a consequence of the heterogeneous elastic-plastic deformation. For instance, for the case of interparticle ligament rupture, the stress intensity between the particles is obtainable from the superposition of the stress induced respectively by the shear stress transfer from the matrix (shear lag) and by the plastic constraint exerted by the particles normal to the direction of the applied stress. The interfacial particle-matrix decohesion, which is generally observed to occur at large plastic straining and the transparticle cracking require consideration of the "back stresses" due to the unrelaxed plastic strain discussed in the preceding section. The superposition of local stresses of various origins will cause local fracture when the local fracture criterion, based on a critical stress or critical strain energy, is satisfied.

(Staff: R. Asaro, J. Fisher, and J. Gurland)

c. Segregant Induced Embrittlement of Grain Interfaces

There are normally ductile materials which exhibit brittle behavior when impurity atoms segregate to their grain interfaces. As a continuation of our earlier work on ductile versus brittle response, conditions were considered under which an interface, possibly containing such an adsorbed species, was capable of sustaining an atomistically sharp cleavage crack rather than having such a crack blunt via dislocation nucleation. In Technical Report 52, two models for ductile versus brittle interface response were examined. One of these was reported earlier by Rice in Technical Report 40, as an extension of his work with Thomson. This approach involved the calculation of the activation energy $U_{act.}$ associated with the nucleation of a metastable loop of dislocation from the tip of a sharp interfacial crack loaded so that Griffith's criterion for cleavage of the interface is just short of being satisfied. If the activation energy is positive, there is a barrier to dislocation nucleation and brittle behavior is expected. Conversely, a negative activation energy would imply dislocation nucleation and thus ductile behavior.

The second model asks the following question: As the crack is loaded and the stress intensity factor is increased, which condition is first reached, a K corresponding to the Griffith load (the crack propagates; brittle behavior) or a K corresponding to a load at which dislocation nucleation is possible (crack blunts; ductile behavior)? The criterion that results is a comparison of two dimensionless parameters, $R_0 \approx (r_0/b)(\gamma_{int}/\gamma_{step})$ and $S \approx \gamma_{step}/\mu b$, (both R_0 and S also depend on orientations) and is given by:

$$R_0^* = \frac{0.58}{S} e^{5S}$$

where R_0^* defines a dividing line between brittle and ductile behavior on the R_0 versus S plane. For a given S, $R_0 > R_0^*$ indicates ductile behavior. Here r_0 is the core parameter, b the lattice spacing, $2\gamma_{int}$ the cohesive energy of the interface, and γ_{step} the effective surface energy of the step formed at the crack tip.

The criterion just described was used as the basis for a model of a grain interface in a face-centered cubic material. The crystalographic orientations of the grains with respect to the interface were assumed to be arbitrary. Individual orientations were modeled by aligning the normal to the interface with a particular direction given in terms of cell edge directions of the fcc lattice. About fifty points, well spaced, on the standard triangle of the $\langle 100 \rangle$ projection were used as test orientations for behavior predicitons using the second criterion discussed above, and including the orientation dependence of R_0 and S.

Data for material properties and experimental observations of brittle versus ductile material behavior were obtained from work by Hondros and McLean (Phil. Mag. 1974) for copper polycrystals containing dilute concentrations of bismuth. In this case, Auger observations of the amount of interfacial segregation of the Bi were available, as were measurements relating to the segregant-induced alterations of surface and grain boundary energies. Our model tends to predict behavior that is generally more ductile than that observed by Hondros and McLean. However, it is important to note that the results are in qualitative agreement, since our model does predict a trend toward brittle behavior as grain boundary energies are lowered by increased segregation of impurity species to the parent interfaces. Reasons for our more ductile behavior include the allowing of unlimited crack line rotation in the model, so that the crack front is assumed always to be in the most favorable position for relaxation by dislocation nucleation before we apply our criterion. Also, the model is not a discrete lattice model and this forces a somewhat arbitrary treatment of dislocation cores and crack tips. A problem arises in determining the step energy γ_{step}. The step occurs in a region of locally heavy segregant concentration and the energy can be estimated only from the surface energies associated with macroscopic-sized surface elements.

Further discussion in Technical Report 52 deals with an analysis of the work of reversible separation of an interface containing a segregated species. This was intended to clarify some issues recently raised in the literature on interfacial embrittlement, especially concerning the distinctions that must be drawn between expressions for cohesive energy reductions for interfacial separation at constant chemical potential, μ, versus separation with constant concentration, Γ, of the adsorbate species. Our conclusion is that despite recent suggestions to the contrary (M.P. Seah, Proc. Roy. Soc., 1975), segregation, even if dilute, does indeed affect the reversible separation of an interface when the separation takes place at constant adsorbate concentration. At the same time, we have verified by specific calculations for a dilute concentration model the general result that the work of separation at constant adsorbate potential μ will, in general, be less than that at constant adsorbate concentration Γ. Further, only the former of these is properly given by an equation of the form:

$$2\gamma = 2\gamma_S - \gamma_b \quad ,$$

as adopted in much of the literature on segregant-induced embrittlement, given interpretations of the kind $\gamma_S = \phi_S$(free energy) $- \mu\Gamma_S$ normally attached to quantities γ_S and γ_b. This form is the correct one for a highly mobile segregant such as hydrogen in certain steels, but not for the segregants associated with the Cu-Bi work discussed and with similar phenomena, e.g. in temper embrittlement of steels by impurities such as those being investigated in our experiments on environmentally affected fractures (see section on Environment Affected Fracture Mechanisms).

(Staff: R.J. Asaro, D.A. Mason, and J.R. Rice)

2. Localization of Plastic Deformation and Inception of Ductile Rupture

The localization of previously homogeneous, or nearly homogeneous, plastic deformation into an intense shear band is a commonly observed precursor to ductile rupture. In some cases the observed localization seems to result as a consequence of the progressive weakening of an alloy due to crack or cavity nucleation at second phase particles. That is, the material becomes progressively more porous until a rupture instability occurs accompanied by intense hole growth to coalescence within the localized zone. In other cases, localization occurs without any direct evidence for incipient cavity nucleation and it presumably results from some instability of the dislocation motion process, which typically leads to cavity nucleation within the localized shear zone. There is also ample evidence for ductile rupture occuring by the growth of holes, nucleated from large inclusions, for which the final joining process is terminated by a shear localization that is, apparently, not directly caused by micro-cavitation but leads to such cavitation, from a smaller and more coherent family of particles for example, carbides in high strength steel or inter-metallic precipitates in aluminum alloys (Cox and Low, Met. Trans., 1974); Van Stone and Psioda, Met. Trans., 1975).

Following our work within the previous grant year (Rice, Technical Report 43, April 1976) on the theory of plastic flow localization, we have begun specific examination of these two mechanisms of flow localization. Thus, for example, by using macroscopic constitutive relations developed previously by Gurson (Technical Report 39, September 1975) for plastically dilatant materials with yielding sensitive to the mean normal stress$[(\sigma_{11} + \sigma_{22} + \sigma_{33})/3]$, McMeeking (Chp. V of Technical Report 48, December 1976) discusses flow localization due to progressive softening of a material by growth of existing cavities, whereas Gurson (Technical Report 46, July 1976) has analyzed the possibility of an instability arising from the rapid nucleation of new cavities over a comparatively narrow range of increasing stress.

Also, Yamamoto (Technical Report 50, April 1977) has examined the sensitivity of localization predictions, based on the Gurson constitutive model, to initial non-uniformities in the volume fraction f of cavities. For mathematical simplicity, the non-uniformity is taken in the form of a planar slice of material with an initial f that differs from that of the surrounding material and the matrix plastic flow is modelled by a pure power law, $\sigma \propto \varepsilon^N$. For example, taking N = 0.1 and assuming a tensile strain at yield of 0.003, the logarithmic strain to localization in plane strain tension, without any accounting for void growth acceleration by triaxiality developed after necking, is predicted to be 0.96 when there is an initial f of 0.01 and no non-uniformity of the void distribution. But with a greater initial f of .03 within the non-uniform slice, the ductility falls to 0.18, and for an initial f of .06, to 0.11. These calculations exhibit a marked sensitivity to material non-uniformities, which we plan to explore further in the coming year. Also, the sensitivity to initial non-uniformities is even greater in axially symmetric tension. Again, in the first calculations which neglect the very important effects of triaxial tension developed in necking, we find for the same N(0.1) and initial f(.01) as above, a predicted ductility near 3 without initial non-uniformities, but this falls to 1.3 for an initial f of .03 within the slice and to 0.6 for an initial f of .06. The calculations done thus far also suggest that for equivalent sized non-uniformities, the ratio of plane strain to axi-symmetric ductility decreases with decreasing hardening exponent N, and this is at least qualitatively consistent with observations by Clausing (Int. J. Fracture, 1970).

Continuing studies by Needleman and Rice are directed to more fully understanding hole growth and nucleation-based ductile rupture instabilities, with special reference to their sensitivity to material non-uniformities and to the development of triaxial stressing.

In addition to studying localization as a consequence of such porosity softening, we have also been concerned with unstabilities of the dislocation motion process per se. These include the instabilities that arise as a consequence of slight pressure sensitivity in the condition for plastic flow (e.g. the "strength differential" effect) and also those which result from triggered mechanisms of plastic flow. The latter include cases, in the context of crystal plasticity, for which stresses other than the Schmid resolved shear stress on a given slip system serve to set up, or "trigger", an increment of plastic flow on that system. Localization arising from such triggered mechanisms has been studied by Asaro and Rice (Technical Report 49, April 1977) with special reference to the onset of cross slip in fcc crystals which seems to fall in this class. Specifically, the effect of the Schmid resolved stress is augmented by the stress component which tends to coalesce the partial dislocations, separated by a stacking fault, that make up a screw dislocation segment, and by the stress component which tends to drive the coalesced segment onto the cross slip plane. For plastic shear on slip planes with normal $\underset{\sim}{m}$ involving dislocations with Burgers vector in direction $\underset{\sim}{s}$, we have assumed that the increment of shear strain is given by

$$d\gamma_{ms} = \frac{1}{h}\left[d\tau_{ms} + \alpha d\tau_{zs} + \beta d\tau_{mz}\right] \qquad ,$$

where $\underset{\sim}{z}$ is the direction perpendicular to $\underset{\sim}{m}$ and $\underset{\sim}{s}$, the τ's are shear stresses, h is the primary slip system hardening rate, and the parameters α and β reflect the non-Schmid effects. We have solved for the critical hardening rate, below which localization occurs, for general anisotropic elastic response in combination with the above plastic response. The results simplify when α and β are small and when the elasticity is isotropic, in which case the critical hardening rate is given by the largest of

$$h_{crit} = \alpha^2\mu/4 \qquad \text{or} \qquad \beta^2\mu/4$$

where μ is the shear modulus and the orientation of the surface of localization is, for the first expression, near the slip plane orientation and, for the second, near the "kink" orientation.

A dislocation model of the cross slip process developed by Asaro and Rice suggests that α is larger than β and, provided that stress levels are large enough for cross slip to be possible,

$$\alpha \approx 0.6/(\partial\tau_1/\partial\tau_{ms})$$

where τ_1 is the concentrated shear stress on the leading dislocation of a pile-up of screw segments and τ_{ms} is the Schmid resolved shear stress. The parameter α increases with decreasing length of representative slip bands; it is of the order 0.1 (within a factor of approximately 2, dependent on the details of slip band geometry) when the band length is 0.1μm and it is smaller by about a third for a length of 1 μm. The predicted h_{crit} of $2.5 \times 10^{-3}\mu$ when $\alpha = 0.1$ is in the range of observed hardening rates at localization and experiments are being begun by Asaro and Chang, under separate funding, to test the theoretical predictions. We have also undertaken some preliminary studies of the role of imperfections in the localization process in single crystals. Although the single slip deformation mode is not nearly as imperfection sensitive as are the cases mentioned earlier, we have noted marked reductions in the strains to localization when the imperfections, modelled after those present in zone hardened crystals, are accounted for in the analysis.

(Staff: R.J. Asaro, A.L. Gurson, R.M. McMeeking, A. Needleman, J.R. Rice, and H. Yamamoto)

3. Mechanics and Mechanisms of Macroscopic Crack Growth and Hole Growth

a) Large Plastic Deformation at a Macroscopic Crack Tip

Technical Report 48, Dec. 1976, by R. M. McMeeking summarized several studies of large crack tip plastic flow and fracture mechanisms in ductile materials. These were in part based on McMeeking's earlier finite element solution (Technical Report 44, May 1976) for the large strain analysis of crack tip opening in elastic-plastic materials under plane strain conditions, and included: models for hole growth and coalescence near a crack tip, analyses of path dependence of the J integral, calculations of energy releases for initial crack growth steps in the large strain region, and comparisons by slip line theory of near tip strain and stress fields for smoothly blunting crack tips and for tips which blunt with the retention of two or more sharp vertices.

The J integral calculations, based on finite element solutions with isotropic hardening incremental plasticity, suggest that the integral is sensibly path independent well within the plastic zone. Path dependence occurs for those paths having radii, as measured in the undeformed reference configuration, which are less than approximately 4 times the crack tip opening displacement in the current, deformed configuration. This supports the use of J as a characterizing parameter for the outer field surrounding the fracture process zone, but also indicates that any conclusions based on evaluation of the integral for paths within the large strain region are likely to be sensitively dependent on the plasticity theory employed (e.g., smooth yield locus/incremental vs. vertex/deformation theories).

The energy releases calculated for finite crack growth steps seem fully consistent with earlier theoretical predictions that the separation energy rate should vanish in the limit of continuous crack growth for elastic-plastic materials. However, the calculations were not carried far enough to study the predictions of stable crack growth that would be implied by the assumption of a critical energy release for rupture associated with small, materially dependent growth steps. This is to be taken up in the portion of the work on the modelling of growing cracks, discussed elsewhere.

McMeeking's comparison of slip line solutions for crack tip blunting with vertices and for blunting with a smooth crack tip confirmed that qualitatively similar near tip behavior results in all cases. This is so in the sense that the triaxial stress elevation typical of plane strain constraint diminishes as the crack tip is approached in the blunting-affected zone, and that large plastic strains develop within that zone. But the details of the strain (and, to a much lesser extent, triaxial stress) distribution is very much dependent on the tip shape assumed. Detailed comparisons for three tip shapes are given in the technical report. Unfortunately, the problem of determining the exact mode of crack tip opening does not have a unique solution from the standpoint of continuum plasticity. Both the vertex and smoothly blunting solutions meet all requisite conditions as mathematical solutions, and the range of deformed crack tip shapes observed experimentally suggests that there is no unique answer at that level either. This non-uniqueness clouds any attempts to model rupture processes in the near tip region and an important problem for the future is to more fully explain those factors which determine the deformed configuration of a crack tip.

(Staff: R. M. McMeeking and J. R. Rice)

b) Computational Elastic-Plastic Analysis of Growing Cracks

Experimental investigations have indicated that for ductile materials under plane strain conditions the inception of crack advance is not necessarily coincident with final fracture. Instead, a regime of stable crack growth is evident in which a crack-containing element may support additional load before the final fracture. Mathematical analyses of the elastic-plastic stress and strain fields accompanying quasistatically extending cracks have, thus far, yielded little detail due to the complexity of the problem. Limiting considerations of these analyses indicate that the strain field pertinent to an extending crack involves a logarithmic plastic strain singularity at the crack tip in contrast to the $1/r$ singularity experienced by a non-hardening stationary crack. The present effort at finite element analysis of the stress and strain fields associated with advancing cracks is described. Also discussed are various macroscopic parameters which have been proposed as correlators of the "state" at an advancing crack tip. Since no technical report has yet been issued on this phase of the work, the description to follow is given in considerable detail.

Numerical procedure: A small strain finite element program is used to investigate the growing crack problem. A crack in an elastic-perfectly plastic material subject to tensile loading is studied under plane strain conditions. The procedure entails following an idealized load-crack advance record which is representative of those encountered in service. The incremental solution is obtained by loading a stationary crack monotonically until the plane strain similarity solution is duplicated, e.g. Tracey (J. Eng. Mat. Tech., Trans ASME 1976), then crack advance stops and further external loading increments are imposed as required by the load-crack growth history to be traced. The stress distributions, the crack face profiles, and various fracture parameters are studied as the crack advances.

As the crack advances through the finite element grid, material directly ahead of the crack tip experiences a change of boundary conditions from displacement controlled to stress controlled. That is, points that had zero displacement conditions due to symmetry have a zero traction condition following crack extension. A nodal release procedure is employed to simulate this change of boundary conditions. When the crack is deemed ready to extend (for the present analysis according to the load crack advance record to be traced), the reaction force equivalent to the zero displacement boundary condition at the crack tip is calculated. This force is then relaxed to zero in a number of steps thereby simulating a stress free crack upon completion of the nodal release process. At present, this procedure is carried out under constant external load and 5 steps of reaction force relaxation are used.

Due to the nodal release procedure used to simulate crack advance, singularity elements are not useful in the present approach. This is because the crack advance would necessitate a refocusing of the singular element configuration at the current crack tip. Since the aim of the analysis is to determine the behavior of the stress and strain fields near a moving crack tip, a high degree of mesh refinement is obligatory. This in turn leads to high computing costs. In an effort to minimize these expenses, the following reassembly and redecomposition techniques were investigated:

i) A procedure devised by Yang (Comp. Meth. in Appl. Mech. and Eng., 1976) was extended to accommodate the purposes of the present analysis. The concept behind this technique involves the numerical extraction of eigenvalue-eigenvector pairs corresponding to altered portions of the master stiffness matrix. Then by performing a sequence of orthogonal transformations utilizing these eigenvalue-eigenvector pairs, the updated stiffness matrix in decomposed form is obtained. For plastic zone sizes involving, say 100 elements, significant savings in reassembly are obtained using this method. A complete description of this method and its merits is contained in a paper by Sorensen (Comp. Meth. in Appl. Mech. and Eng., 1977).

ii) out-of-core assemblers and decomposers were also investigated. These procedures seek to minimize the core requirements of the finite element analysis and rely on the high speed information transfer rate of peripheral drums and disks to effect cost savings. The tradeoff here is core storage costs versus input-output costs. This procedure was not found to be competitive with the in-and-out of core procedures described next.

iii) in-and-out of core procedures were found to be cost optimal for the reassembly and redecomposition of elements with altered moduli when the number of such elements exceeded about 150 elements. Here, the degrees of freedom associated with the changing element stiffnesses were placed at the end of the degrees of freedom array so that only a small portion of the master stiffness matrix needs reassembly and redecomposition. The reassembly stage is done in core with storage requirements specified only for the nonzero components of the altered stiffness matrix. Then the out-of-core redecomposition procedure is employed. The advantage this procedure enjoys over the complete out-of-core procedure is that the in-core condensed assembly eliminates many input-output steps and requires a small amount of core since it treats only nonzero terms of the altered stiffness.

Of course, the above conclusions are strictly true only for the particular computer configuration and peripheral equipment available at Brown and the specific grid employed in this analysis, but the trend of these large scale computing results may serve as a guideline for future analyses. Some results of the crack growth modelling for an ideally plastic material are summarized now.

Crack face profiles: Plots of the crack face profiles at various stages of the load history reveal a displacement distribution that seems to be consistent with previous theoretical studies (Rice, Treatise on Fracture, 1968). In particular, a crack tip advancing in steady state conditions is predicted to have a displacement distribution proportional to $r \ln r$, where r is distance measured from the crack tip. This dependency implies a vertical tangent at the crack tip, a feature which appears consistent with the numerical solution. The consequences of this are that the proposed material dependent fracture parameter known as the crack tip opening angle (e.g. Andersson, J. Mech. Phys. Solids 1973), is not well defined at the crack tip. However, the vertical tangent is a local effect and may not overwhelm a defined crack tip opening angle. For example, the present results indicate that values of 0.0074, 0.0081, 0.0084, 0.0086, and 0.0087 radians are obtained following the five nodal release steps when the crack tip opening angle is defined as the arc tangent of the vertical displacement of the node immediately behind the crack tip divided by the appropriate horizontal distance. The above progression of values indicates approach to steady state conditions, but the physical meaning of such a parameter is clouded by the vertical tangent present at the crack tip.

Stress fields: Results for the stress fields accompanying the extending crack indicate that material points ahead of a growing crack experience effectively the same stress elevations observed ahead of a stationary crack in plane strain tension. Microstructural consequences of this observation are that fracture mechanisms for the onset of growth, such as the cracking and decohesion of second phase particles from matrix material due to the high stress elevations remain operational during quasistatic crack advance. There may be some more significant differences for materials with strong strain hardening and this is left to future work. After the crack has passed a material point, unloading of the σ_{yy} stress occurs and σ_{xx} becomes the dominant stress. A thin band of actively yielded "wake" material is observed behing the advancing crack tip. This material is yielding with σ_{xx} as the driving stress.

Plastic zone shapes: Following the first nodal release step, the "butterfly" plastic zone shape familiar from static crack solutions is constricted and is tilted towards the symmetry axis ahead of the advancing crack tip. Upon further loading at constant crack length, the static shape is somewhat restored. Crack advance steps and external load incrementation steps repeat the cycle of constriction and tilting upon crack advance and attempted restoration of the static shape upon further loading. The amount of restoration achieved depends on the number of increments associated with the load incrementation at constant crack length. A thin bond of yielded elements trails the crack tip throughout the constriction-tilt-restoration cycle of the plastic zone. It should be noted that detailed analytic and numerical analyses of extending cracks in anti-plane strain exhibit a similar cycle of plastic zone shapes.

Separation energy rates: Each nodal release step provides a trend of vertical displacement versus reaction force. Calculating the area under this curve and dividing by the finite crack advance step one obtains the separation energy rate, G^{Δ} in the notation of Kfouri and Rice (Fracture, 1977). It is the finite value of the crack advance step that permits this calculation, for in the limit of crack advance step approaching zero and for materials which exhibit a finite stress level at the crack tip such a calculation is well known to lead to zero for the separation energy rate. The steady state G^{Δ} value obtained from the present analysis may be contrasted with similar values obtained by Kfouri and Miller (Proc. Inst. Mech. Eng. 1976) for the plane strain analysis of center-cracked plates under various modes of loading. By plotting these points appropriately, relationships between G^{Δ} and the J integral are derived. What is evident from these relations is that the use of J as a correlator of separation energy rates during a finite growth step is highly sensitive to the non-singular terms present in the stress expansion at the tip of a plane strain crack (e.g., Rice, J. Mech. Phys. Solids, 1974). This result underlines the lack of a macroscopic parameter that successfully correlates with the crack tip stress and strain state during crack growth.

More detailed discussions of all the above results form part of a Ph.D. thesis under preparation by Sorensen.

(Staff: A. Needleman, J. R. Rice, and E. P. Sorensen)

c) Numerical Analysis of Fully Plastic Flow

A new finite-element method has been developed for dealing with fully incompressible material behavior under plane strain conditions. The requirements for this type of analysis arise in a number of ductile fracture models, e.g., those involving hole growth under creep and more-or-less rate independent plastic conditions.

In this method groups of simple elements are arranged into "superelements" so that the incompressibility constraints are satisfied within each superelement. These superelements are then used as the building blocks in the finite element grid. The advantages of this approach for the type of problems envisioned here are: (i) most of the work done in imposing the incompressibility constraints can be done once at the beginning of a calculation and need not be repeated at each stage of a nonlinear solution procedure, (ii) the resulting stiffness matrices are positive definite (and symmetric). The bandwidth of these matrices is increased compared with that for the corresponding problem for a compressible material, but the order is reduced.

A computer program has been written implementing this algorithm and several model problems solved. The results have been most encouraging regarding both the accuracy and efficiency of this approach and a report describing this work is in the process of being written. The current version of the program incorporates power law hardening material behavior and, for materials undergoing steady state creep, can accommodate large deformation.

(Staff: A. Needleman)

d) Experimental Evaluation of Surface Toughness by Indentation Cracking

The method consists of measuring incrementally the specific work required for the propagation of surface cracks in brittle materials due to high load hardness indentations. A possible use is as a simple measure of surface toughness, but the relation between the surface toughness and the fracture toughness has not been unequivocally established on the basis of fracture mechanics.

An empirical study was carried out as an undergraduate project. It demonstrated the feasibility of meaningful indentation cracking provided that residual surface stresses were minimized by mechanical polishing and heat treatment. An empirical correlation could be shown to exist between experimentally determined surface fracture toughness and bulk fracture toughness, but only an order of magnitude agreement was found between the measured fracture toughness and several theoretical models based on bulk fracture toughness. (Ref: B. R. Lawn and R. Wilshaw, J. Mat Sci., 10 (1975) p. 1049-1081).

(Staff: E. Exner and J. Gurland)

4. Environment-Sensitive Fracture Mechanisms

The past and recent literature has provided many examples of environmentally induced or assisted fractures in the form of "hydrogen embrittlement", "temper embrittlement" and stress corrosion cracking. Many of these phenomena apparently do not involve a change in fracture mode, but rather seem to bring about the normal process of fracture, as would occur in the absence of the environment, at lower stresses and strains. This is the case, for example, in the ductility losses observed in low and medium strength alloys when they are exposed to hydrogen containing environments. Alternatively it happens, especially in higher strength materials, that the environment will induce a change in fracture mode from a ductile hole initiation and growth sequence to more brittle processes such as transgranular or intergranular cleavage. Thus in the first case adverse environments seem mainly to accelerate hole initiation (or even possible growth) while in the second case the environment allows more brittle, less energy consuming, events to set in rather early in the deformation-fracture process.

Now since the beginning stages of most fracture processes in metals, whether it be the initiation of voids leading to ductile fracture or the initiation and growth of brittle cracks, involves separation or decohesion along internal interfaces of some sort, it is natural to attempt to quantify the effect of an environment on interfacial separation. This is the subject of much of our theoretical study on interfacial cohesion and ductile-brittle response (section 1c) and our experimental program is designed to be as complimentary to this effort as is possible.

Our proposal of last year was to study hydrogen assisted fractures in various medium and high strength steels, initially in environments of dry hydrogen gas and later in aqueous media. The specific materials we have selected are a 4140 high strength steel and an HY-130 medium strength steel. We have designed and are constructing sets of rather novel environmental chambers which are used to contain the notched section of our four-point bend (i.e. pure bend) and compact tension specimens. These chambers are "O" ring sealed to the specimens and allow for tension-compression (or bending) motion by using flexible stainless steel bellows. Hydrogen is introduced into the specimen chamber after evacuation through a palladium diffusion filter which assures purification of the gas. From the experiments we expect to attain an understanding of the effects of hydrogen on (i) accelerating hole initiation in front of blunt notches and sharp cracks, (ii) accelerating the coalescence of holes through perhaps premature localized shearing, and (iii) inducing transitions in failure mode from ductile to brittle.

In order to study the effect of hydrogen on a single brittle mode of fracture, we have obtained from the Bethlehem Steel Corp. several plates of a 4140 steel, each with carefully controlled phosphorus levels. The alloys with high impurity levels will be heat treated to induce intergranular temper embrittlement and then tested in hydrogen. Our preparatory work is now nearly complete and we plan to perform much of the experimental work this summer.

During the development period outlined above, we have been conducting a study of the effect of hydrogen on ductile fractures in plain carbon spheroidized steels. Hydrogen has been introduced by cathodic charging under varying conditions of imposed current density and time of exposure. So far our results for two steels (viz. 1.05 and a 0.45 wt percent C) indicate that the effect of hydrogen on the process of particle-matrix separation itself is actually very small even though we observe substantial ductility losses as measured by area reductions at fracture. The appearance of the fracture surfaces for the hydrogen charged and the uncharged steels is similar, e.g. a roughly equivalent dimple size, and this again suggests that the effect of hydrogen on initiating voids at the particles is small. On the other hand, we have noted throughout our study of void formation at particles that an important part of the fracture initiation process in such steels involves interfacial cracking. After the voids are formed it is common that they propagate as fine cracks along interfaces, either grain or subgrain boundaries, and usually link up with other cracks propagating from above or below. Those cracks then open laterally, especially in the hydrostatically stressed region in the specimen's center, to form larger holes which enter directly into the fracture process. It has occurred to us that hydrogen, if it lowers the strength of these boundaries (e.g. by the mechanisms suggested in section 1), may have the effect of accelerating this process of boundary fracture by reducing the local stresses or the hydrostatic tensions, which are developed by increased necking, required to propagate the cracks. The effect is, in any event, rather subtle and is being investigated further. We plan to complete this stage of our work on particle cavitation in hydrogen environments this summer by conducting tests on a 1045 steel which has been heat treated to produce microstructures with and <u>without</u> subgrain boundaries and which has a range of grain sizes. Control of these variables should help to understand the boundary effects. Finally, in order to understand how hydrogen influences void initiation and fracture ahead of cracks and notches in these low strength steels, we are also testing cathodically charged deeply notched four-point bend specimens. This work is currently in progress and will also be completed this summer.

(Staff: R. Asaro, H. Cialone and J. R. Rice)

B. Reports, Publications, Theses, Oral Presentations, and Other Related Activities

1. Technical Reports

C00-3084-45	Progress Report, July 1976.
C00-3084-46	A.L. Gurson, Porous Rigid-Plastic Materials Containing Rigid Inclusions-Yield Function, Plastic Potential, and Void Nucleation (July 1976).
C00-3084-47	J.R. Rice, Elastic Plastic Fracture Mechanics (September 1976).
C00-3084-48	R.M. McMeeking, Large Plastic Deformation and Initiation of Fracture at the Tip of a Crack in Plane Strain (February 1977).
C00-3084-49	R.J. Asaro and J.R. Rice, Strain Localization in Ductile Single Crystals (May 1977).
C00-3084-50	H. Yamamoto, Conditions for Shear Localization in the Ductile Fracture of Void Containing Materials (May 1977).
C00-3084-51	Y.W. Chang, Bauschinger Effect and Workhardening in Spheroidized Steels (May 1977).
C00-3084-52	D. Mason, Segregation Induced Embrittlement of Grain Interfaces (May 1977).

2. Publications

*L. Anand and J. Gurland, Strain-Hardening of Spheroidized High Carbon Steels, Acta Metallurgica, (1976) 24, P. 901-909.

R.J. Asaro and J.R. Rice, Strain Localization in Ductile Single Crystals, submitted to J. Mech. Phys. Solids.

D.K. Brown and R.M. McMeeking, A Finite Element Analysis of a Circumferentially Notched Tensile Specimen, in Fracture 1977 (Proc. 4th Int. Cong. Fracture), ed. D.M.R. Taplin, University of Waterloo Press, Vol. 3, 1977, pp. 507-513.

Y.W. Chang and R.J. Asaro, Bauschinger Effects and Work-Hardening in Spheroidized Steels, submitted to Met. Trans.

*A.L. Gurson, Continuum Theory of Ductile Rupture by Void Nucleation and Growth: Part I, Yield Criteria and Flow Rules, Trans. ASME (Jour. Engr. Materials and Technology), Vol. 99, 1977, pp. 2-15

A.L. Gurson, Porous Rigid Plastic Materials Containing Rigid Inclusions--Yield Function, Plastic Potential, and Void Nucleation, in Fracture 1977, (Proc. 4th Int. Cong. Fracture), ed. D.M.R. Taplin, University of Waterloo Press, Vol. 2, 1977, pp. 357-364

R.M. McMeeking, Blunting of a Plane Strain Crack Tip into a Shape with Vertices, Trans. ASME (Jour. Engr. Materials and Technology)--in press.

R.M. McMeeking, Finite Deformation Analysis of Crack Tip Opening in Elastic-Plastic Materials and Implications for Fracture Initiation, Jour. Mechanics and Physics of Solids--in press.

R.M. McMeeking, Path Dependence of the J Integral and the Role of J as a Parameter Characterizing the Near Tip Field, ASTM Special Technical Publication (Proc. ASTM 10th National Symp. on Fracture Mechanics, August 1976)--in press.

S.P. Rawal and J. Gurland, Fracture Initiation at a Macroscopic Crack Tip in Spheroidized Carbon Steels, Proceedings 4th Int. Congress on Fracture, University of Waterloo, Canada, D.M.R. Taplin, Editor, (1977) Volume 2, P. 41.

S.P. Rawal and J. Gurland, Observations on the Effect of Cementite Particles on the Fracture Toughness of Spheroidized Carbon Steels, Metallurgical Transactions (1977) Vol. 8A, P. 691-698.

*S.P. Rawal and J. Gurland, Observations on the Effect of Cementite Particles on the Fracture Toughness of Spheroidized Carbon Steels, Proceedings of 2nd Int. Conf. on Mechanical Behavior of Materials, Am. Soc. Metals, Metal Park, Ohio, (1976) P. 1154-1158.

J.R. Rice, Elastic-Plastic Fracture Mechanics, in The Mechanics of Fracture (ed. F. Erdogan), Applied Mechanics Division, Vol. 19, ASME, New York, 1976, pp. 25-53.

*J.R. Rice, The Localization of Plastic Deformation, in Theoretical and Applied Mechanics, (Proc. 14th Int. Cong. on Theor. and Appl. Mech., Delft, 1976), ed. W.T. Koiter, Vol. 1, North-Holland, 1976, pp. 207-220.

*Previously listed as "in press"

3. Theses (All degrees awarded in June, 1977)

Y.W. Chang, Sc.M., May 1977, Bauschinger Effects and Work-Hardening in Spheroidized Steels.

D. Mason, Sc.M., May 1977, Segregation Induced Embrittlement of Grain Interfaces.

R.M. McMeeking, Ph.D., November 1976, Large Plastic Deformation and Initiation of Fracture at the Tip of a Crack in Plane Strain.

H. Yamamoto, Sc.M. , April 1977, Conditions for Shear Localization in the Ductile Fracture of Void Containing Materials.

4. Oral Presentations

R. Asaro presented a seminar talk on work related to strain localization and fracture in single crystals at McMaster University (April 1977). He also presented a lecture on this same subject at the Spring Meeting of AIME (March 1977) and will be presenting an invited lecture at the Fall Meeting of AIME (October 1977).

J.R. Rice gave the opening lecture ("Theory of Ductile Fracture") at the British Metals Society Fracture Workshop, University of Glasgow, August 1976. He also gave the invited sectional lecture on plasticity (The Localization of Plastic Deformation) at the 14th International Congress on Theoretical and Applied Mechanics., Delft, August 1976. In addition, Rice gave a survey lecture on "Elastic-Plastic Fracture Mechanics" at the Symposium on the Mechanics of Fracture, ASME Annual Meeting, New York, November 1976, gave a seminar of the same title at Washington University, St. Louis, March 1977, and gave a U.S. Steel Research Laboratory Lecture on "Plastic Flow Localization and the Inception of Ductile Rupture", Monroeville, June 1977.

E.P. Sorensen gave seminars on "Some Numerical Studies of Stable Crack Growth" at the General Motors Technical Center, Warren, April 1977, and at the Ford Research Laboratories, Dearborn, May 1977.

S.P. Rawal presented his and Gurland's work on fracture of steels at the 2nd International Conference on Mechanical Behavior of Materials, Boston, Massachusetts, July 1976 and at the 4th International Congress on Fracture, Waterloo, Canada, June 1977.

5. Related Activities

R. Asaro organized a symposium on the "Fundamental Aspects of Plasticity and Fracture" at the Fall meeting of the AIME in Niagara Falls, New York.

R. Asaro gave the special topics course entitled "Environmental Effects in Mechanical Behavior" at Brown during the second semester of the 1976/77 academic year. Professors Rice and Gurland participated in the lectures and discussions.

J. Gurland organized an NSF Workshop on Hard Materials in June 1977 at Brown University, which dealt in part with strength and fracture toughness of tool materials.

C. Personnel

1. Personnel Connected with Contract

1. Professional Staff: R.J. Asaro, J. Gurland, A. Needleman, and J.R. Rice

2. Research Engineer: L. Hermann

3. Technical Assistant: H. Stanton

4. Research Assistants (Graduate Students): Y.W. Chang*, H. Cialone, J.R. Fisher, D. Mason, R.M. McMeeking* E.P. Sorensen*, A. Tin**, and H. Yamamoto**

5. Undergraduate Research Assistant: E. Exner*

*Supported for portion only of contract period
**Not supported by contract

2. Present Positions of 1976 Graduates

R.M. McMeeking, Ph.D., 1976, Acting Assistant Professor, Department of Mechanical Engineering, Stanford University.