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

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R. J. Asaro, J. Gurland, A. Needleman and J. R. Rice

Division of Engineering

Brown University

Providence, Rhode Island

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Summary of Significant Accomplishments

Recent progress was achieved in refining and generalizing the methods previously developed for treating the stable crack growth problem, with particular attention to the approximate asymptotic solution of Rice, Drugan and Sham for stress and deformation fields near the tip of a growing crack.

The microstructural aspects of ductile fracture were studied in dual-phase steels and high-strength 4340 steels. In the latter, it was found that material toughness, as measured by ductility, is reduced with increasing austenite grain size, whereas crack growth at a sharp pre-fatigue crack, as in the K_{IC} test, is more difficult with larger grain sizes. The cause of this difference is being investigated further.

Very interesting results were obtained in the work on hydrogen effects in steels. In medium strength steels, the ductility-reducing effect of hydrogen is tentatively attributed to the accumulation of hydrogen at internal interfaces with a resulting loss in the resistance to interfacial separation. The suggested mechanism is quite similar to that previously attributed only to the brittle intergranular fracture of high-strength steels.

Extension of Needleman and Rice's work on the growth of cavities at elevated temperatures to the investigation of the effects of triaxial stressing relates the rate of void growth by grain boundary diffusion and dislocation creep to the triaxiality. It provides a good model to analyze the growth of macro-cracks in polycrystals by the mechanisms of growth and coalescence of micro-voids. Other useful results pertaining to elevated temperature rupture processes were obtained from the

examination of the effects of non-steady loading on the generation of internal stress concentrations at creep cavities.

Table of Contents

- A. Detailed Description of Research Program
 - 1. Elastic-Plastic Analysis of Stable Crack Growth
 - 2. Microstructural Aspects of Fracture Processes in Ductile Alloys
 - a) Deformation and fracture in ductile two-phase alloys
 - b) Correlation of microstructure with fracture toughness in high strength steels
 - 3. Environmentally Assisted Fracture Mechanisms
 - 4. Elevated Temperature Rupture Processes
- B. Reports, Publications, Oral Presentations, Theses and Degrees Awarded
- C. Personnel Connected with Contract

A. DETAILED DESCRIPTION OF RESEARCH PROGRAM

1. Elastic-Plastic Analysis of Stable Crack Growth

Our effort to attain a fundamental understanding of and to provide an analytical description for elastic-plastic crack growth in ductile metals, by closely coordinating analytical, numerical finite element and experimental investigations, has continued. Much of our recent progress has constituted refinements and generalizations of the methods developed in recent years under this contract to treat the stable crack growth problem. The work of Rice, Drugan and Sham (ASTM STP 700, 1980, pp. 189-221) provided an approximate asymptotic solution for stress and deformation fields near the tip of a growing crack, which was coupled with a numerical finite element study to evaluate parameters undetermined by the asymptotic analysis; this solution was coupled with a fracture criterion proposed in the earlier work of Rice and Sorensen (J. Mech. Phys. Solids 26, 1978, pp. 163-186) to yield a fairly complete description of stable crack growth in elastic-ideally plastic solids under small scale yielding conditions.

The asymptotic solution presented in the Rice, Drugan and Sham study was an approximate one, which made the assumption that the full three-dimensional von Mises yield condition could be replaced, in angular plastic sectors as the crack tip is approached, by the simpler condition that the in-plane maximum resolved shear stress must attain the value of the material's shear strength, τ_0 , for plastic response:

$$\left(\frac{\sigma_{\theta\theta} - \sigma_{rr}}{2} \right)^2 + \sigma_{r\theta}^2 = \tau_0^2 \quad (1)$$

This is a reasonable assumption since the three-dimensional von Mises yield condition does reduce to this form in asymptotic plastic sectors

which produce singular strain; thus it is only an approximation in plastic asymptotic sectors which do not produce singular strain.

A recent analytical investigation by Rice (Rodney Hill 60th Anniversary Volume, Pergamon Press, Oxford; expected publication May, 1981) develops the formulation for the exact elastic-ideally plastic asymptotic analysis of growing plane strain cracks. This formulation employs the full three-dimensional form of the yield condition in non-singular asymptotic plastic sectors, giving four differential equations which govern the four unknown stress components, one of these equations being the compatibility condition since stress fields in such sectors are not statically determinate.

The Rice study extends the concepts developed initially for asymptotic solution of crack problems in specific limited classes of material behavior, while developing a unified approach to treat asymptotic analysis of cracks growing under any of the three fracture modes. Whereas previous formulations were restricted to cracks in isotropic elastic-ideally plastic solids satisfying either Tresca or von Mises yield conditions, the present approach encompasses the general class of elastic-ideally plastic solids permitting arbitrary material anisotropy and arbitrary yield condition form, provided that the flow rule is of the associated type (normality) and that the material is homogeneous. Among the significant results of the study, centered fan sectors of singular straining at the crack tip are shown to be a general feature of the large class of material response treated, as are also the plastic strain singularity types associated with stationary and growing cracks.

Employing this general formulation by Rice of the governing equations for a near-tip plastic sector which does not produce singular strain,

Drugan and Rice developed an exact asymptotic solution of the stress and deformation fields near a growing crack (the full three-dimensional form of the von Mises yield condition is used). The manuscript detailing this solution is currently being prepared for publication. A solution was obtained for Poisson ratio 0.3, and this solution confirmed the accuracy of the approximation of assuming Eq. (1) to hold in all angular plastic sectors as the crack tip is approached. The asymptotic configuration of the exact solution resembles the modified Prandtl field approximate solution of Rice, Drugan and Sham quite closely: the differences are that the plastic sector bordering the crack flank in the exact solution is a non-singular plastic sector instead of a constant stress sector, and the angles of the elastic wedge boundaries in the exact solution are $\theta_1 = 109.95^\circ$ and $\theta_2 = 159.84^\circ$, where θ is measured from the line ahead of the crack.

The rate of crack opening for the exact solution is given by an expression of the same form as that originally proposed by Rice and Sorensen,

$$\dot{\delta} = \alpha \dot{J} / \sigma_0 + \beta (\sigma_0 / E) \dot{a} \ln(R/r) \quad (2)$$

where J is the far-field value of the J -integral, σ_0 is yield strength, E is the elastic modulus and a is crack length. For Poisson ratio 0.3, the exact asymptotic solution gives $\beta = 5.447$; α and R are undetermined by the asymptotic analysis.

Another result of the Rice study and the Drugan and Rice analysis was to find an error in the approximate analysis of Rice, Drugan and Sham: namely, although their expressions for velocities and strain rates in a moving centered fan section have the correct forms, the coefficients

they gave are incorrect. These slight errors arose due to a tricky limit calculation: since $S_{rr} \rightarrow 0$ and $S_{33} \rightarrow 0$, and thus $S_{\theta\theta} \rightarrow 0$, in a centered fan sector, and since plastic strain rates are given by

$$D_{ij}^p = \Lambda S_{ij},$$

(where S_{ij} are deviatoric stresses and $\Lambda \geq 0$ is an initially undetermined parameter), Rice, Drugan and Sham, as did Rice and Sorensen, assumed that all of D_{rr}^p , $D_{\theta\theta}^p$ and $D_{33}^p \rightarrow 0$ as $r \rightarrow 0$. As shown in the Rice study, this is not the case; rather, all of D_{rr}^p , $D_{\theta\theta}^p$ and D_{33}^p are singular of order $e_2 \dot{a}/r$ as $r \rightarrow 0$ (since Λ turns out to be sufficiently singular that, e.g., $\Lambda S_{rr} \neq 0$ as $r \rightarrow 0$). This error means that the values of θ_1 , θ_2 and β given by Rice, Drugan and Sham for $\nu = 0.3$ are not the correct results of the approximate asymptotic analysis; thus, Drugan and Rice also reworked the approximate asymptotic analysis (which assumes validity of (1) in all plastic sectors as $r \rightarrow 0$), correcting this error of Rice, Drugan and Sham, finding for $\nu = 0.3$ that $\theta_1 = 110.22^\circ$, $\theta_2 = 161.04^\circ$ and $\beta = 5.460$. Comparison of these results to those quoted above for the exact solution verifies the accuracy of this approximate asymptotic analysis.

Although uniqueness of the exact near-tip configuration cannot be proved, the accuracy of the approximate solution would appear to justify the assumption, for the purpose of examining alternate possible solution configurations, that Eq. (1) holds in plastic sectors as the crack tip is approached. Such an examination was made: many logical alternate configurations were postulated and analyzed to see if all governing equations and boundary conditions could be satisfied. The result of this lengthy procedure was that within the approximate formulation

characterized by the assumption of Eq. (1) in asymptotic plastic sectors, no solution other than the modified Prandtl field, as discussed above, could be found.

Finite element calculations for the growing crack under small scale yielding conditions are continued. The implementation of the finite element procedure as outlined in last year's Technical Progress Report has been completed. The essence of this finite element procedure is to represent the stress and displacement fields in the far field elastic region, which is defined to remain elastic throughout the deformation history, by a convergent series in the far field in terms of some unknown coefficients. The inner region near the crack tip which undergoes elastic-plastic response is discretized into finite elements in the usual manner. The far and inner fields are coupled by requiring that the displacements at finite element nodes for these two fields be the same along their common boundary. Thus the potential energy functional for the union of the far and inner regions can be expressed readily in terms of the unknown coefficients and the finite element nodal displacements inside the inner region (excluding those on the common boundary of the two regions). The potential energy functional is then minimized with respect to these two sets of unknowns and upon eliminating the unknown coefficients, there results a set of finite element equilibrium equations with the nodal displacements inside the inner region as unknowns. The resulting stiffness matrix is symmetric and positive-definite and the usual finite element solution scheme can be employed to solve this set of non-linear equations. Two elastic solutions were carried out for the types of loadings and configurations shown in Figure 1.1 as test cases. The coefficients as predicted from the numerical calculations

are compared with their theoretical values; quite close agreement is found as shown in Table 1.1. Also, a 4-noded constant dilatation element developed by Nagtegaal, Parks and Rice (Comp. Meth. Appl. Mech. Engr., 1974) is used in the present calculation in order to relieve the artificial "mesh locking" effect under nearly incompressible conditions. The computation is currently underway.

A different finite element investigation, with the purpose of elucidating near-tip fields as conditions progress from small scale to large scale and finally general yielding, is being carried out. The specific problem under investigation is a deeply-cracked bend specimen comprised of elastic-ideally plastic material deforming under plane strain conditions. The main goals of the calculations are the determination of the dependence, if any, of the parameters α , β and R in the theoretical crack opening rate equation (2) on the extent of yielding, and to determine an appropriate definition for J in this expression. The eventual objective of these determinations is to enable employment of the theoretical growth equation of Rice and Sorensen, obtained by integrating the opening rate expression (2), for general extents of yielding.

The geometry being analyzed corresponds closely to the specimens tested experimentally by Hermann and Rice (Met. Sci., Aug.-Sept. 1980) to facilitate comparison of the results with experimental behavior. The initial ligament size and the specimen height are $0.174 W$ and $1.5 W$ respectively, where W is the width of the specimen.

Four-noded constant dilatation elements are also used in this calculation as the artificial "mesh locking" effect mentioned earlier would be more pronounced under large scale and general yielding conditions.

Displacements corresponding to a rigid rotation, $\frac{\theta}{2}$, together with a rigid vertical translation of unknown magnitude are prescribed on the finite element nodes on the top and cracked side of the specimen. It is observed that the forces, which are not known a priori, required to produce these prescribed displacements on the boundary do no work on a rigid translational deformation field. Thus, we can eliminate this unknown rigid displacement and obtain a set of finite element equilibrium equations for the displacements inside the body (excluding those along the boundary where displacements are prescribed). The resulting stiffness matrix is symmetric and $\frac{\theta}{2}$ can be treated as a monotonically increasing load parameter. A test case was carried out by loading the specimen up to the fully plastic range with the crack being stationary. A limit moment, as would be expected with the deployment of the four-noded constant dilatation element, was obtained from the numerical solution. However, it is about 4% higher than the value of the classical limit moment of Green and Hundy. Crack growth under continuous loading is simulated by releasing incrementally the nodal restraining force at the crack tip while simultaneously increasing the load. These calculations are being carried out.

Preliminary experiments on HY-130 steel were conducted, utilizing pre-fatigued compact tension specimens and employing the highly accurate differential compliance technique developed earlier under this contract and described in last year's Technical Progress Report to measure amounts of stable crack growth. The methodology was the same as that of Hermann and Rice, and the experiments were specifically gauged to supplement and expand the Hermann and Rice work by providing data for stable crack growth

far into the fully yielded range, while testing a steel more suitable to structural applications. (The steel tested by Hermann and Rice, an AISI 4140, was chosen exclusively for its property of providing extensive stable crack growth in the small scale yielding range, thus facilitating assessment of our theoretical growth predictions.) The plan is to compare the new experimental results with the aforementioned numerical finite element analysis of the same geometry in the large scale and general yielding range, with the goal of analytically characterizing stable crack growth over the full range of yielding. The recent experiments provided data for stable crack growth with yielding far into the fully plastic range, most of the crack growth occurring under such full yield conditions. As done by Hermann and Rice, the experimental data were used to determine plots of the "deformation theory" value of the J integral, J_d , versus crack length a , for each specimen. Although little of the measured crack growth occurred in the small scale yielding range, this portion of the J_d vs a curves was seen to agree well with the analytical small scale yielding predictions. The phenomenology of the experimental results beyond the contained yielding range is quite different: among the trends noted are that the J_d versus a curves show an initial decrease in slope as general yield is attained (a feature also in evidence in the Hermann and Rice results), but as crack growth continued a marked increase in this slope was consistently noted. Interpretation of this behavior should be facilitated by the numerical finite element study described above, and the testing of other steels, as proposed, will be initiated when interpretation of these preliminary studies has been made. Also, since our overall objective is the

characterization of stable crack growth over the entire range of small scale through general yielding, future testing will be conducted on HY-130 which has been heat-treated to reduce J_{IC} and hence to provide significant amounts of stable crack growth in all ranges of plastic yielding.

(Staff: R. J. Asaro, J. R. Rice, W. J. Drugan, T. L. Sham, S. Tse and L. Hermann)

Semi-infinite elastic sharp crack with crack tip at $z = c$ under mode I loading and plane strain conditions.

Semi-infinite elastic sharp crack loaded by two point forces P on the crack surfaces under plane strain conditions.

Figure 1.1

<u>Coefficients</u>	<u>Finite Element Solution</u>	<u>Exact Solution</u>
a_1	$-9.2475639 \times 10^{-2}$	-9.396298×10^{-2}
a_2	$-1.0729102 \times 10^{-2}$	-1.106556×10^{-2}
a_3	$-2.5279392 \times 10^{-3}$	-2.606275×10^{-3}
a_4	$-3.9915094 \times 10^{-4}$	-7.673209×10^{-4}
a_5	$-3.5669961 \times 10^{-4}$	-2.530182×10^{-4}

- Coefficients for the problem of a semi-infinite elastic sharp crack with crack tip at $z = c$ under mode I loading and plane strain conditions. $K_I = 1$, $c/R = 0.471$.

$$\sigma = \frac{K_I}{\sqrt{2\pi r}} \tilde{f}(\theta) + \frac{a_1}{r\sqrt{r}} \tilde{f}_1(\theta) + \frac{a_2}{r^2\sqrt{r}} \tilde{f}_2(\theta) + \dots$$

$$+ \frac{b_1}{r^2} \tilde{g}_1(\theta) + \frac{b_2}{r^3} \tilde{g}_2(\theta) + \dots$$

<u>Coefficients</u>	<u>Finite Element Solutions</u>	<u>Exact Solution</u>
a_1	$-2.1215025 \times 10^{-1}$	-2.120443×10^{-1}
a_2	3.1434736×10^{-2}	3.136594×10^{-2}
a_3	$-8.3220465 \times 10^{-3}$	-8.351464×10^{-3}
a_4	2.5556492×10^{-3}	2.647205×10^{-3}
a_5	$-6.7659849 \times 10^{-4}$	-9.136842×10^{-4}

- Coefficients for the problem of a semi-infinite elastic sharp crack loaded by two point forces P on the crack surfaces under plane strain conditions. $P = 1$, $c/R = 0.4437$.

Table 1.1

2. Microstructural Aspects of Fracture Processes in Ductile Alloys

a) Deformation and fracture in ductile two-phase alloys

Work has begun on the study of deformation and fracture of dual-phase steels. The dual-phase steels are low carbon steels heat treated to produce a structure consisting of ferrite and martensite. These steels are of tremendous interest to the automotive industry because of the weight-saving potential associated with high strength and good formability. They are also of great scientific interest because they represent the class of ductile two-phase alloys with variable and controllable amounts of the hard phase (martensite) embedded in a ductile matrix (ferrite). This study is a logical extension of our previous work on particle strengthened alloys, such as the spheroidized steels.

An important difference between spheroidized steels and dual-phase steels is the relative amount of the hard phase that each contains. Whereas the spheroidized carbon steels generally contain less than 20 volume percent of cementite, the dual-phase steels generally contain 15-30 percent of martensite, and they can be produced experimentally with martensite contents up to 90 percent. With large amounts of the hard phase, the load carried directly by the hard particles cannot be ignored and the process by which the load is transferred to the particles should be considered in any hardening theory.

The first part of this study is concerned with an estimate of load transfer in a dual-phase steel at yield. The extent of load transfer is calculated by extension to irregular particles of the shear lag mechanism developed for discontinuous fibers (A. Kelly, Strong Solids, 1966). The model has been previously presented (J. Gurland, *Scripta Met.*, 1979, Vol. 13, pp. 967-969). The load transfer is proportional

to a measure of the aspect ratio of the hard particles, i.e. the ratio between the average caliper length of the particles $\bar{D}_\beta$, in the direction of loading, and the mean intercept length $\bar{L}_\beta$. Assuming linear load transfer between the ductile matrix and the non-deforming particles, one obtains

$$R_\sigma = \frac{\bar{D}_\beta}{\bar{L}_\beta} + 1$$

for the ratio of the stresses in the two-phases. The theory was applied at yield to a dual-phase steel (Jones and Loughlin, Steel Co., VAN-QN, .12C, 1.63 Mn), with a measured yield strength of 47.0 ksi. From the model, the calculated stresses in ferrite and martensite were 39.2 ksi and 88.1 ksi, respectively, with $R_\sigma = 2.2$.

In the same steel, we measured the diamond penetration hardness (DPH) of the alloy and the microhardness of the ferrite. Because of the experimental difficulty in obtaining microhardness values at very low indenter loads (5-20g), and the lack of clear-cut theoretical correlation between hardness and stress under the indenter, only a very tentative result was obtained which gives $R_H = 1.9-2.7$ for the stress ratio during indentation. Nevertheless, the results support at least qualitatively the role of load transfer as a significant strengthening mechanism in two-phase alloys, in addition to the matrix hardening processes usually considered.

This work is described in Technical Report No. 83, June 1981.

In the second part of this study, we examined the plastic deformation and fracture of the VAN-QN steel. The ductile ferrite matrix phase deforms by slip from the very beginning of plastic deformation. Slip

lines were not observed in the martensite at any strain. Plastic elongation of the martensite particles was noted only in the center part of the neck, i.e. at strains of the order of 0.9. The evidence for martensite particle deformation was obtained by measurement of the particles' average aspect ratio.

Void formation is due to decohesion of the interface between martensite particles and ferrite grains, and not to particle cracking. It is observed that void initiation occurs most frequently between closely-spaced martensite particles along grain boundaries, especially between the particles grouped in planar arrays or bands. The void formation was studied by optical microscopy and scanning-electron-microscopy (SEM) of longitudinal sections and fracture surfaces.

A quantitative study was undertaken of the void density distribution as a function of distance from the minimum cross-section. It is found that the void density is a function of strain, and, for that reason, the void density increases markedly in the necked region.

Further analysis is in progress. Generally, the observation of fracture in dual-phase steels appears to be in excellent agreement with the experimental and theoretical trends found by J. Fisher in recent work on spheroidized steels (Technical Report No. 77, April 1980). A Sc.M. thesis by A. Szewczyk is in preparation.

(Staff: R. J. Asaro, J. Gurland and A. Szewczyk)

b) Correlation of microstructure with fracture toughness in high strength steels

In our last two Progress Reports we discussed our work correlating microstructure with fracture toughness in high strength 4140 and 4340 steels. The important microstructural features that were controlled in both steels were prior austenite grain size, martensite packet size and, indirectly through tempering, carbide size and distribution. Our results for 4140 steel (e.g. Technical Report 67) showed that prior austenite grain size and martensite packet size were extremely important for determining toughness and ductility, but that the phenomenology was rather complex and in some ways unexpected. For example, it was found that ductility and impact energies decreased as grain size increased, whereas K_{IC} values increased with increasing grain size. This phenomenology is identical to that reported earlier in the literature for a variety of similar ultra-high strength steels. Earlier attempts in the literature to explain this behavior made use of the now well known idea that in order for a crack to advance it must produce a critically intense stress-strain field over a critically large enough distance within the microstructure. This idea has led to a very successful phenomenological description of cleavage in mild steels where cleavage is known to initiate from isolated carbides on ferrite grain boundaries (Technical Report 20). The situation in martensitic steels is, of course, much more complicated but these ideas may still retain merit as a basis for describing the fracture process. In our previous work on 4140 steel, for example, the critical microstructural unit was thought to be the mean martensite packet size and using this we had showed that K_{IC} did scale with packet size.

In order to further explore the correlation between austenite grain size, martensite packet size and fracture toughness, and in particular to better understand the curious role of austenite grain size on fracture toughness, we initiated a novel study on grain refined 4340 steels. In cooperation with Mr. George Vandervoort of the Bethlehem Steel Corporation we had prepared several heats of 4340 steel which were grain refined with Al, Zr and Ti. The results with Zr-killing were not successful in producing a tough steel. Our results with Ti-killing were indeed very successful and the resulting microstructures provided a good correlation with the Al-killed steel. Figure 2.1 shows plots of austenite grain size and mean colony size vs. austenitizing temperature. The steel labeled "K" was Ti-killed and that labeled "16" was Al-killed. For austenitizing temperatures up to 1100°C the austenite grains were of uniform size; above 1100°C the austenite grain size became non-uniform and, at 1200°C consisted of a bimodal distribution of fine and coarse grains. Thus, for austenitizing temperatures up to at least 1100°C , the Ti- and Al-killed steels allowed for comparisons of the qualitative effects of austenite grain size, and martensite colony size, on toughness.

Figure 2.2 shows data on ductility and true fracture stress vs. austenitizing temperature. The more significant losses in reduction in area and fracture stress occur in the Al-killed steel which underwent significant grain coarsening. The Ti-killed steel underwent only a modest loss in ductility and fracture stress consistent with its modest grain growth. This effect on ductility, which was similar to the effect on toughness, demonstrates a loss in overall material toughness with increasing grain size. Figure 2.3 shows data on plane strain fracture

toughness, K_{IC} , vs. austenitizing temperature which shows the effect in question. The Al-killed steel displayed a nearly two-fold increase in K_{IC} with increasing grain size, while the Ti-killed steel showed only a very slight increase, again consistent with the modest increase in grain size in this steel. It is difficult to extract from this data possible separate effects of colony size and austenite grain size, but the data clearly indicates that K_{IC} does not increase with austenitizing temperature unless the austenite grain size increases.

The use of higher austenitizing temperatures was found to lead to a more refined carbide size and spacing in both the Al-killed and Ti-killed steels. There did not appear to be a significant difference in carbide morphology between the two steels except that the carbide spacing in the Ti-killed steel was somewhat smaller than in the Al-killed steel. This, in turn, may have had some effect on the process of void initiation. The fracture modes in the two steels were very similar except at the highest austenitizing temperatures (i.e. 1200°C) where the Al-killed steel displayed increasing amounts of intergranular fracture. In terms of the micro-mechanisms of fracture, it should be pointed out that the inclusions seem to play a very minor rôle in both steels. In fact, the total inclusion content, which was similar for both steels, was less than 0.20 percent by volume; the sulfide content was lower in the Ti-killed steel which also had about 0.05 percent Ti bearing inclusions.

The results described above again suggest that it is important to consider the particular stress-strain field in which a crack is to initiate in order to evaluate toughness. On the one hand it appears

evident that material toughness, as measured by ductility for example, is reduced with increasing austenite grain size, while crack growth at a sharp pre-fatigue crack, as in the K_{IC} test, is more difficult with larger grain sizes. The exact mechanism of crack initiation is not clear as yet and is the object of our ongoing research. The appearance of the fracture surfaces suggest that the martensite packet size is important since, where regions of quasi-cleavage existed, the size of the facets was comparable to the packet size. However, there are other possibilities that warrant study as well. For example, 0.40 percent carbon is commonly listed as the carbon content above which plate martensite (twinned) forms rather than lath martensite (dislocated). Twinned martensites are less ductile and so, if it were to happen that large grain sizes promote twinned vs. dislocated martensites in our steels, this may help explain the reduced ductility accompanying increases in austenite grain size. The trends in K_{IC} values on the other hand can only be understood with a more detailed description of the crack initiation process at a sharp crack and so continued studies are currently underway to study this further. One set of experiments to be performed involves metallographic observations of crack initiation beneath sharp cracks. Future work is described more thoroughly in our renewal proposal.

(Staff: R. J. Asaro, J. Gurland and L. Majno)

Figure 2.1

Figure 2.2

Figure 2.3

3. Environmentally Assisted Fracture Mechanisms

Of the many ways in which hydrogen can degrade the mechanical properties of materials, two, in particular, seem most prevalent in steels: hydrogen either causes a change in the mode of fracture, usually from a "normally" ductile process involving void initiation and growth, to less ductile transgranular or intergranular cleavage, or hydrogen enhances, without changing the character of the "normal" mode of failure. The first instance is common in high strength steels where ductile fractures are often found to give way to cleavage presumably brought on by a relaxation of a local fracture stress (or strain) due to hydrogen segregation and accumulation at internal interfaces. In high strength alloys that would normally display cleavage fracture, possibly due to the prior embrittling effects of impurities, for example, hydrogen can have the second effect and enhance a "normal" intergranular or transgranular cleavage by lowering even further the stresses required locally to cause failure.

Our studies on hydrogen assisted fracture in three spheroidized steels, described below, represent examples of where hydrogen does not alter the fracture mode, which in this case is ductile, but accelerates it with strain. On the other hand, as the hydrogen content was increased in our two lower carbon steels there was a transition in fracture mode from void initiation and growth to transgranular cleavage. Another example of this type is represented by our study of hydrogen assisted fracture of a high strength 4140 steel where transitions in fracture mode are common. In the experiments to be described in this area, our steels were purposely temper embrittled so that the effects

of hydrogen on a single fracture mode could be studied in a quantitative manner.

a) The role of hydrogen in medium strength steels

Our study of the effects of hydrogen on the fracture of plain carbon spheroidized steels has been completed with the publication of two new papers (Met. Trans. 1981, and Proceedings of the Third Conference on the Effects of Hydrogen on Material Behavior). In these studies three steels were used, viz. a 1045 and a 1017 plain carbon steel, and a 0.15 weight percent carbon steel. All three steels had spheroidized microstructures, but in the 1017 steel, both the grain size and the average carbide particle size were varied in order to further study the effect of microstructure on hydrogen assisted ductile fracture. The results in all three steels showed that hydrogen had the effect of accelerating void initiation at inclusions and cementite particles and of accelerating void growth particularly along grain boundaries. Both effects contributed to accelerated (i.e. with strain) ductile fracture and a loss in ductility.

Our earlier results for the 1045 steel indicated that hydrogen had the effect of accelerating both void initiation and void growth, but did not change the nature of the fracture process which was by ductile void initiation and growth. The effect of hydrogen on void initiation was quantified by adapting and refining somewhat the method introduced by Argon et al. (Met. Trans. 1975) which attempts to measure a critical interfacial normal stress to cause cavitation. With hydrogen this critical interfacial stress was found to be approximately 550 MN/m^2 , while without hydrogen the critical stress was found to be approximately 950 MN/m^2 . Void growth, which was also accelerated by hydrogen, was found to be quite interesting. Voids grew along ferrite grain boundaries and

developed in size faster than would be expected from plasticity controlled growth. This was true, in fact, with and without hydrogen and thus illustrated, in a novel way, an important contributing mechanism to ductile void growth. Thus aside from facilitating void initiation, hydrogen accelerated void growth along interfaces leading to earlier internal crack formation, ductile rupture and a loss in ductility.

In the lower carbon steels the phenomenology was somewhat more complicated in that as the hydrogen content was increased there was a change in the fracture mode from one of void growth and coalescence to one involving transgranular cleavage. The onset of cleavage was associated with a severe loss in ductility as shown in Figures 3.1 and 3.2 for two steels and four microstructures in the 1017 steel. Steels A-E are described in Table 3.1. One important difference between Steel B (actually microstructure B), and microstructures C and D, is that microstructures C and D are much finer, both in terms of grain size and particle size. Microstructure E had a finer particle size than B but a coarser grain size--its behavior was intermediate between microstructures B and C, D. Our results led to a model, a part of which is illustrated in Figure 3.3. The model states that microstructures containing more total interface, which in turn act as sinks for hydrogen, will contain less hydrogen dissolved in the iron lattice or, for that matter, at any given interface such as inclusion-matrix interfaces. Such microstructures will be less prone to cleavage which was found to initiate predominantly at inclusions. This model is still somewhat tentative, but it provides a simple and consistent rationale for the observed phenomenology. When fracture was entirely by ductile void

growth we found that, again, void initiation was facilitated by hydrogen. Void growth took place along interfaces, viz. grain boundaries, and possibly sub-grain boundaries. Void growth was accelerated by hydrogen in much the same manner as in the 1045 steel.

The results of the present study suggest a kind of explanation for the commonly observed ductility losses in hydrogen containing environments that is more in the spirit of models which have until now been exclusively associated with brittle intergranular fracture of high-strength steels-- that is the accumulation of hydrogen at internal interfaces with a resulting loss in the resistance to interfacial separation.

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

b) Hydrogen effects in the cracking of high strength steel

While most steels demonstrate some susceptibility to hydrogen assisted fracture, as described for example in the previous section, high strength steels seem to be particularly sensitive. The very high stress levels, especially beneath notches and cracks, and the particular microstructures in these steels lead to crack initiation at carbides or inclusions after only very limited plastic straining. Hydrogen appears to have the adverse effect of lowering the cohesive strength at internal interfaces (e.g., particle-matrix interfaces), as well as of the iron lattice itself, and thereby facilitating crack initiation. The present study was aimed at quantifying the effect of hydrogen on the initiation of fracture in a high strength 4140 steel. In order to simplify the fracture process the steels were purposely temper embrittled so as to

avoid transitions in fracture mode; in this condition the fractures, with or without hydrogen, would be by intergranular cleavage.

The approach taken was based upon the phenomenological idea that cleavage fracture initiates when critically high stresses or strains prevail over critically large distances in the microstructure. The critical distances are linked to the spacing of potential crack initiating sites in the microstructure, such as carbides or inclusions, and the critical stresses or strains are those needed to initiate and drive microcracks from the initiating sites to a main crack, or between initiating sites. This approach has proven quite useful in analyzing cleavage fractures in steels in air. For example, as discussed earlier, in a high-nitrogen mild steel, the temperature dependence of the critical stress intensity, K_{IC} , over the range 123K (-150°C) to 198K (-75°C) has been successfully predicted by noting the behavior of the uniaxial yield stress and the hardening properties over this range of temperatures. The predicted K_{IC} values were closest to the actual K_{IC} values when the so-called "characteristic distance" was set equal to two grain diameters. This distance corresponded closely with the spacing of grain boundary carbides which were found to initiate cleavage. Similarly, in spheroidized plain carbon steels with a range of carbon contents, the average critical distance was determined over the temperature range 75K (-198°C) to 123K (-150°C); this distance was equal to 1.3 times the ferrite grain size.

The purpose of the present study was to identify the fracture initiating feature of the microstructure, thus determining the critical distance (δ^*), and to measure a critical stress (σ^*) on specimens tested

in air or in gaseous hydrogen. The ultimate goal was to use these measurements to predict the threshold stress intensity K_{TH} (i.e. the stress intensity below which, for the hydrogen pressure used, no cracking occurs, regardless of the time of exposure), and to compare it to the value measured on an actual fracture toughness test conducted in hydrogen. As just mentioned, to this end, the 4140 steel specimens were previously temper embrittled so as to avoid the complications involved in the fracture mode transition that would otherwise occur. In this way, it was possible to study, in a quantitative manner, the effect of hydrogen on a single fracture mode, namely intergranular cleavage.

Bend tests were conducted at room temperature in ultra-high purity hydrogen. The specimens had a notch geometry identical to the one analyzed by Griffiths and Owen and were loaded in 4-point bending. The environmental chamber, containing the notched section of the specimen, was alternately evacuated and purged with argon to remove as much oxygen as possible, thereby facilitating the adsorption of hydrogen onto the specimen. The evacuated chamber was then backfilled with hydrogen to a pressure of 1 atm, allowing the specimen to "soak" for several hours. Loading was then done incrementally with hold times ranging from 1h to 48h between load increments to allow the internal hydrogen activity (or concentration) to at least approach equilibrium with the local stresses. When cracking was detected by an acoustic emissions transducer, the chamber was purged with argon and then opened, and the split-pin wedges were inserted into the specimen. Upon unloading, during which the opening displacement was generally well maintained, the notch was filled with an infiltrating epoxy for the purpose of edge

retention during polishing. The section containing the notch was cut out and then sectioned perpendicularly to the notch plane. This section was then metallographically polished, etched and examined both optically and in the scanning electron microscope (SEM). The position at which cracking initiated below the notch was identified, and the conditions for crack initiation were determined.

In addition to the bend tests conducted in the hydrogen chamber, in-situ experiments were conducted in the SEM on thin wedge-loaded specimens using a device built by J. Hong and J. Gurland at Brown. These specimens, resembling compact tension specimens, were tested to observe deformation and cracking on the polished and etched surface in an effort to understand the process in the interior of the thicker bend bars. The specimens were U-notched with a notch root radius equal to that of the four-point bend specimens; the notch was again aligned parallel to the short-transverse plane. Figure 1 contains a series of SEM micrographs from one of these specimens. The figure shows the sequence of events, consisting of delamination and cracking of MnS inclusions, which lead to crack formation and growth with increasing force applied by the wedge. In the early stages of deformation, most of the sulfides in the vicinity of the notch delaminate and in the process often crack; one of these eventually emerges as the primary fracture initiating site at which a crack forms and then propagates through the specimen. Crack growth seems to take place along prior austenite grain boundaries and, to some extent, lath boundaries. While cracks usually initiated at sulfides, some crack initiation was observed in regions where no inclusions were apparent. This occurred at much higher loads than did crack initiation at sulfides, at regions of intense strain.

The events leading to subsurface cracking in the bend bars (bent in air or in hydrogen) were found to be qualitatively the same as those just described for the thin wedge-loaded specimens, except that in the bend tests cracks always initiated at sulfides. Presumably this is because the tests were stopped as soon as cracking was detected, when throughout the specimen the stresses were too low to cause cracking anywhere except at sulfides. In fact, due to the extreme brittleness of this steel (even without hydrogen), many specimens fractured completely within moments of the detection of subsurface cracking. This factor, combined with the necessary use of several specimens in the calibration of the acoustic emissions system and the limited supply of steel, resulted in a very small number of successful tests. Once the subsurface crack was revealed by polishing and etching, its precise position below the notch was determined so that the local conditions for crack initiation could be determined. The finite element solution of Griffiths and Owen for an elastic-plastic material was used to analyze cracking in specimens tested in air. In many instances, the specimens tested in hydrogen exhibited cracking at loads at which there was essentially no plastic deformation. For these cases the elastic solution of Neuber was employed. The local maximum principal stress necessary for crack initiation at inclusions is given in Table 3.2 for all successful tests. While the critical stress values for type "b" inclusions (i.e. those aligned perpendicular to the rolling direction) in plate 2 (tested in hydrogen) indicate that these values are dependent on the hold time, the values of the critical stress for type "a" inclusions (i.e. those aligned parallel to the rolling direction) for hold times of 1h vs. 48h suggest that any differences

may be attributable to experimental scatter inherent in the testing technique. This limited sampling indicates that increasing the hold time from 1h to as much as 48h has no effect on the critical stress for cracking at inclusions. Thus the kinetics of hydrogen adsorption, absorption and diffusion to highly stressed regions are such that in less than 1h the hydrogen activity (or concentration) is nearly in equilibrium with the local stress field. This is supported by the fact that when cracking did occur, it was detected within 1/2 h of the load increment.

As Table 3.2 indicates, crack initiation at type "a" inclusions was easier in plate 1 than in plate 2. One possible explanation for this difference is that Mo, acting as an anti-segregant, causes inclusions in plate 2 (containing more Mo than plate 1) to have fewer embrittling impurities at the inclusion-matrix interface than do inclusions in plate 1. By virtue of their orientation with respect to the local applied stress, type "a" inclusions require higher stresses to delaminate than do type "b" inclusions. However, since type "a" inclusions are not potential fracture initiating sites, the conditions leading to their delamination and cracking are not particularly relevant here.

With the fracture initiating sites identified and the critical conditions for cracking at these sites determined, it should be possible to predict K_{TH} in 1 atm of hydrogen. It would seem reasonable to take the spacing between type "b" inclusions (directly below the notch) as δ^* and the critical stress for cracking at these inclusions as σ^* . Thus, for both plates δ^* would be approximately 800 μm , and σ^* would be 690 MPa (100 ksi) for plate 1 and 1180 MPa (170 ksi) for plate 2.

Upon studying the stress distribution ahead of a crack tip, it is immediately obvious that these criteria lead to unrealistically large values of K_{TH} . In point of fact, when fracture toughness tests were performed in 1 atm of hydrogen on pre-fatigue cracked bend bars (using K_I increments of $2.2 \text{ MPa}\cdot\sqrt{\text{m}}$ ($2 \text{ ksi}\cdot\sqrt{\text{in.}}$) with hold times of 2h), K_{TH} was $35 \text{ MPa}\cdot\sqrt{\text{m}}$ ($32 \text{ ksi}\cdot\sqrt{\text{in.}}$) for both plates. This represents a roughly 55 pct reduction in toughness as compared to an identically heat treated 4140 steel with a similar chemical composition (Technical Report 67). More significantly, although σ^* for plate 2 was some 70 pct greater than σ^* for plate 1, K_{TH} was the same for both plates. This implies that the sulfides do not play a major role in cracking ahead of a sharp crack. Even when thin layers were consecutively ground off, polished, etched and inspected, no interaction between inclusions and the growing crack was observed. Evidently, cracking ahead of the sharp crack occurred elsewhere within the microstructure, possibly by cracking and delaminations of smaller carbide particles on prior austenite grain or martensite lath boundaries. Since this event was never observed in the notched specimens, a σ^* for this type of fracture initiating site was not measured in these experiments. In the notched bend bars, with stress distributions much broader than those in the pre-cracked specimens, the probability of finding a type "b" inclusion in the most highly stressed region of the specimen is relatively high, simply because this region usually extends some two to three notch root radii below the notch. The pre-cracked specimens, on the other hand, had a stress distribution which dropped off much more rapidly, so that the probability of stressing an inclusion enough to cause cracking at the inclusion before a

crack could initiate in the matrix is quite low. Thus, as was sometimes observed in the latter stages of deformation in the wedge-loaded specimens, crack initiation occurred elsewhere in the intensely stressed region near the crack tip. Correlations between cracking behavior in notched specimens with notch root radii as large as is standard in a Charpy bar and in specimens with initially sharp cracks would therefore seem to be inappropriate, or at least ambiguous. A similar situation was encountered in a study of the effect of prior austenite grain size on fracture in air, where the fracture toughness as measured by standard Charpy V-notch impact testing could not be directly correlated to toughness measurements made on pre-cracked compact tension specimens. This has been discussed in Section 2b. The authors felt that the steeper stress gradient ahead of a crack (as compared to that of a notch) caused the compact tension specimens to require a higher stress intensity to critically stress larger prior austenite grains, resulting in an increase in K_{IC} which was not indicated by the impact tests.

It is clear that in the present instance, the critical distance δ^* is not fixed by the microstructure, but is in fact also affected by the loading conditions and by microstructural variations. Although cracking can and does initiate at certain sites in the steel matrix, such as at fine carbide precipitates at prior austenite grain and martensite lath boundaries, it occurs more easily at MnS inclusions. Therefore, when the stress distribution is broad, cracks will usually initiate at these inclusions, and they will be the fracture controlling feature of the microstructure. On the other hand, when the stress distribution is quite narrow, as in the case of a sharply cracked specimen, and the

inclusion content is relatively low, the crack initiating sites in the matrix will usually be stressed highly enough to cause cracking at these sites rather than at inclusions. Under these conditions δ^* might be equal to the prior austenite grain size or martensite lath colony size. What is needed to resolve this problem is an exhaustive study of cracking in both notched and pre-cracked specimens. Thus, matrix-associated cracks could be observed in the notched bars and inclusion-associated cracks could be observed in pre-cracked bars, and the type of connection attempted herein could be made.

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

TABLE 3.1
MICROSTRUCTURAL DIMENSIONS AND STRENGTH LEVELS.

<u>Steel</u>	<u>Grain Size</u>	<u>Particle Diameter</u>	<u>Yield Strength</u>
A-1015 (tempered 250 hrs.)	14 μm	0.9 μm	331 MN/m^2 (48 ksi)
B-1017 (tempered 24 hrs.)	9.0 μm	1.0 μm	248 MN/m^2 (36 ksi)
C-1017 (tempered 1 hr.)	4.2 μm	0.4 μm	269 MN/m^2 (39 ksi)
D-1017 (cycled 1 hr.)	4.4 μm	0.4 μm	295 MN/m^2 (43 ksi)
E-1017 (austenitized 1 hr. at 1323 K, then tempered 1 hr.)	11 μm	0.4 μm	317 MN/m^2 (46 ksi)
1045	4.7 μm	1.9 μm	435 MN/m^2 (63 ksi)

TABLE 3.2

Critical Stress for Crack Initiation
at Sulfide Inclusions

<u>Plate 1</u>	<u>Type "a"</u>	<u>Type "b"</u>
In air	-	2215 MPa (320 ksi)
atm H ₂ (1h hold time)	-	690 MPa (100 ksi)
 <u>Plate 2</u>		
In air	-	2630 MPa (380 ksi)
atm H ₂ (1h hold time)	1380 MPa (200 ksi)	1245 MPa (180 ksi)
atm H ₂ (24h hold time)	-	1105 MPa (160 ksi)
atm H ₂ (48h hold time)	1520 MPa (220 ksi)	-

Figure 3.1 The loss in RA (non-uniform reduction in area) at fracture for steels A through E vs. charging current density, as compared to the uncharged condition.

Figure 3.2 Fraction of fracture surface exhibiting quasi-cleavage fracture features vs. charging current density for steels A through E.

Figure 3.3 (a) An MnS inclusion in a stressed specimen (hydrogen charged), slightly inclined to the tensile axis. Some delamination of the inclusion-matrix interface has begun to occur. (b) With additional stress, the inclusion breaks with the two sections aligning themselves with the tensile axis. A small crack forms in the space between the sections. (c) The crack then grows in a brittle manner as shown schematically. The micrograph shows a typical crack of this type which has closed to a large extent upon unloading. (d) Schematic representation of a developing "fisheye" which was formed by steps a, b and c.

Figure 3.4 Crack initiation in a wedge-loaded specimen by delamination of an MnS inclusion, with subsequent early stages of growth. The notch orientation is approximately horizontal.

4. Elevated Temperature Rupture Processes

Needleman and Rice's work (Acta Met. 28, 1315 (1980), referred to as NR) on the growth of cavities along grain interfaces by the combined processes of grain boundary diffusion and dislocation creep in the adjoining grains has provided a full analysis of these complicated coupled processes under tensile loading conditions. NR, following the idea of Beere and Speight (Metal Sci. 12, 172 (1978)) have shown that the principal effect of the deformability of the adjoining grains is to shorten the diffusion path along the grain boundary from the inter-void half-spacing b to a distance of order L ahead of the void. This is true at least when $a+L$, where a is the void radius, is less than b . Here L , defined as

$$L \equiv (D\sigma/\dot{\epsilon}_{cr})^{1/3}$$

is a stress and temperature dependent parameter, having dimension of length, introduced by Rice, where $\dot{\epsilon}_{cr}$ is the creep rate of the adjoining grains due to stress σ .

NR's studies have been extended to the investigation of the effects of triaxial stressing. These effects would occur, for example, in front of macro-cracks or notches where materials experience elevation in hydrostatic stress. The understanding of the influence of this hydrostatic stress elevation on the void growth rates, under conditions at which the diffusion and creep processes are coupled, is particularly important in the modelling of macro-crack growth in polycrystals by the mechanisms of growth and coalescence of micro-voids.

The finite element method as developed by NR was used to analyze this problem. For detailed discussion of the finite element formulation,

see NR. To fix ideas, consider an array of voids on a grain boundary perpendicular to the direction of tensile loading. This cavitated grain boundary is subjected to a remote loading $\sigma_{zz\infty}$ in the tensile direction and $\sigma_{rr\infty}$ in the radial direction. This situation can be modelled by considering a right circular cylinder of material with a void at the center. Since the geometry and loading considered are axisymmetric in nature, the analysis reduces to that of a two-dimensional problem. The void is assumed to be of spherical-caps shape. This is justifiably so if the surface diffusion is rapid enough that a quasi-equilibrium void shape is retained. For the effects of non-equilibrium void shape, see the work of Chuang, Kagawa, Rice and Sills (Acta Met. 27, 265 (1979)).

The grains are modelled as incompressible and assumed to obey a power law creep constitutive law of the form

$$\sigma = \Lambda \dot{\epsilon}^{1/n}$$

in uniaxial tension where Λ and n are constants. For brevity, the field equations and boundary conditions for the problem on hand are summarized in Fig. 4.1, where σ_{∞} and $\dot{\epsilon}_{\infty}$ are Mises equivalent stress and strain rate, respectively. In Fig. 4.1, the radial velocity on the cylinder wall is taken to be uniform and equal to the remote field in order to simulate the constraint of adjoining materials. Also, on the grain boundary, matter conservation and kinetic relation for diffusion have to be satisfied. Of course, the void surface is traction-free.

The numerical solutions of the axisymmetric void growth model under triaxial stressing were carried out for various values of a/L starting from one limit where the diffusion process dominates (i.e., a/L small),

through the intermediate range where the coupling between diffusion and creep is important, to the other limit where the creep process controls (i.e., a/L large). For each fixed value of a/L , the influence of the hydrostatic stress on the void growth rates was also explored. The normal stress σ_o acting on the grain boundary at the void tip was taken to be zero for all cases considered, and a representative value of 5 for the hardening exponent n was assumed. The results are summarized in Fig. 4.2, where the non-dimensional volumetric growth rates $\dot{V}/(a^3 \dot{\epsilon}_\infty)$ are plotted versus σ_m/σ_∞ for various values of a/L . The non-dimensional parameter, σ_m/σ_∞ , where σ_m is the mean normal stress, is a measure of the triaxiality. For example, in front of a plane strain macro-crack, σ_m/σ_∞ is 2.383 for non-hardening materials and is 4.243 for power law hardening materials with $n=5$. The factor P appearing in Fig. 4.2 is a scaling factor which enables all the cases considered to be plotted on the same graph.

In order to place the results shown in Fig. 4.2 in a better perspective, it is helpful to consider the effects of triaxiality on the void growth rates for the two limiting cases. First, if the diffusion process on the grain boundary is the dominant mechanism, the grains are effectively rigid (Hull-Rimmer model), so that the volumetric growth rate is (NR):

$$\frac{\dot{V}_{rg}}{a^3 \dot{\epsilon}_\infty} = \frac{2\pi}{(a/L)^3} \left[\frac{\frac{\sigma_m}{\sigma_\infty} + \frac{2}{3} - (1-a^2/b^2) \frac{\sigma_o}{\sigma_\infty}}{\ln(b/a) - (3-a^2/b^2)(1-a^2/b^2)/4} \right] \quad (1)$$

Thus the volumetric growth rate increases linearly with the triaxiality in this limit. On the other hand, if the stresses are high and the creep

flow is rapid enough that grain boundary diffusion can be neglected, Budiansky et al.'s result ("Mechanics of Solids, The Rodney Hill 60th Anniversary Volume," edited by Hopkins et al., Pergamon Press, 1981) for a spherical void in power law creeping materials under triaxial stressing can be modified slightly to give

$$\frac{\dot{V}_{cr}}{a^3 \epsilon_{\infty}} = 2\pi h(\psi) \left[\alpha_n \frac{\sigma_m}{\sigma_{\infty}} + \beta_n \right]^n . \quad (2)$$

when σ_m/σ_{∞} is greater than 1 .

Here $\alpha_n = 1.5/n$, $\beta_n = (n-1)(n+0.4319)/n^2$ and $h(\psi) = \left(\frac{1}{1+\cos\psi} - \frac{\cos\psi}{2} \right) / \sin\psi$, where $h(\psi)$ is a function of the void tip half angle ψ and it accounts for the fact that the void is not a sphere as was considered by Budiansky et al. This result indicates that the volumetric growth rate increases as a power of the triaxiality in this creep limit.

From Fig. 4.2, it can be seen that the volumetric growth rates behave as predicted in the diffusion ($a/L = 0.01$) and creep ($a/L = 10$) limit. For intermediate values of a/L , the volumetric growth rates increase linearly with the triaxiality at the early stage, then increase very rapidly at high levels of triaxiality. The triaxiality level $(\sigma_m/\sigma_{\infty})_{crack}$ experienced by a material point in front of a plane strain macro-crack in power law hardening materials is marked on the graph in Fig. 4.2. The results indicate that this rapid increase in the volumetric growth rates is substantial at this level of triaxiality for intermediate values of a/L at which diffusion and creep processes are coupled.

In order to represent the results shown in a quantitative manner, we first note that based on an observation of Dr. I. W. Chen of M.I.T.

(privately communicated by Professor A. S. Argon to Professor J. R. Rice), a reasonable approximation to NR's results for tensile loading is to predict the volumetric growth rate from Eq. (1), but to use the maximum of $(a/b)^2$ and $(a/(a+L))^2$ instead of $(a/b)^2$. This approximation leads to the prediction of volumetric growth rates to within an error of about 30% of NR's results for all values of a/L less than 10.

When there is triaxial stressing, guided by the present numerical results, we have found that a reasonable approximation to the volumetric growth rate is

$$\frac{\dot{V}}{a^3 \dot{\epsilon}_\infty} = \frac{2\pi}{(a/L)^3} \left[\frac{\left(\frac{\sigma_m}{\sigma_\infty} + \frac{2}{3} \right) - (1-f) \frac{\sigma_o}{\sigma_\infty}}{\frac{1}{2} \ln \left(\frac{1}{f} \right) - (3-f)(1-f)/4} \right] + 2\pi h(\psi) \left[\alpha_n \frac{\sigma_m}{\sigma_\infty} + \beta_n \right]^n \quad (3)$$

where $f = \max\{(\frac{a}{b})^2, (\frac{a}{a+\gamma L})^2\}$ with $h(\psi) = 0.61$ for $\psi = 70^\circ$ and γ is a numerical factor. The accuracy of this approximation is shown in Table 4.1 for various values of γ . We can see that when $\gamma = 1.25$, the approximation gives results that are within 22% of the numerically computed values. It should be noted that for all computations, σ_o was assumed to be zero; however, based on the approximation to NR's results for tensile loading, Eq. (3) is expected to apply for non-zero values of σ_o .

From Eq. (3) we can write the void growth rate as

$$\frac{\dot{a}}{a \dot{\epsilon}_\infty} = \frac{1}{(a/L)^3 h(\psi)} \left[\frac{\left(\frac{\sigma_m}{\sigma_\infty} + \frac{2}{3} \right) - (1-f) \frac{\sigma_o}{\sigma_\infty}}{\ln \left(\frac{1}{f} \right) - (3-f)(1-f)/2} \right] + \frac{1}{2} \left[\alpha_n \frac{\sigma_m}{\sigma_\infty} + \beta_n \right]^n \quad (4)$$

with $f = \max\{(\frac{a}{b})^2, (\frac{a}{a+1.25L})^2\}$.

This relates the void growth rate to the triaxiality and provides a good model to analyze the growth of macro-cracks in polycrystals by the mechanisms of growth and coalescence of micro-voids in front of the main crack.

Another area of interest in our investigation of elevated temperature rupture processes is the examination of the effects of non-steady loading on the generation of internal stress concentrations in solids of high temperatures. Grain boundaries containing creep cavities in materials subject to cyclic and rapidly-applied loading are analyzed. The response of partially damaged materials (where damage is represented as crack-like cavities on the grain boundaries) following load alterations at low stress levels (low enough not to produce any significant plastic deformation) and at temperatures near $0.5 T_m$ have been investigated. The interaction between grain boundary diffusion and elastic deformation is important under these conditions. The damage process is caused by material redistribution from the void surfaces to the grain boundaries. The main matter-transporting mechanisms are surface and grain boundary diffusion. The same mechanisms dominate in the stress relaxation process.

To analyze the stress field on the grain boundaries, a coupled elasticity-diffusion problem is considered. The formulation of the boundary value problem for the elastic stress field, which is constrained to satisfy the grain boundary diffusion and transport conservation equations on the grain boundary, and to obey stress-free conditions at the crack-like cavity surfaces, has been described in the Progress Report for the previous period (ending June 1980).

The normal stress σ , acting on the grain boundary and the effective "thickening" δ , satisfy

$$D \frac{\partial^2 \sigma}{\partial x^2} + \frac{\partial \delta}{\partial t} = 0, \quad (5)$$

where t is time, x is position along the grain boundary, and $D = D_b \delta_b \Omega / kT$. Here $D_b \delta_b$ is the grain boundary diffusion coefficient, Ω is the atomic volume, and kT is the energy per atom measure of temperature. The analysis is based on the concept of representing a crack as an array of continuously distributed opening dislocations along the grain boundary; here the dislocation density is time-dependent. We address for simplicity the case of plane strain deformation with an effectively infinite grain boundary. The governing coupled elasticity and diffusion equations take the form:

$$\sigma(x, t) = \sigma_{\infty}(t) - \frac{E}{4\pi(1-\nu^2)} \int_{-\infty}^{\infty} \frac{\partial \delta(x', t) / \partial x'}{x - x'} dx', \quad (6)$$

$$\frac{\partial \delta}{\partial t} + D \frac{\partial^2 \sigma}{\partial x^2} = r(x, t).$$

Here $\sigma_{\infty}(t)$ is the time-dependent applied stress, $r(x, t)$ is an effective rate of matter supply, and for simplicity we have taken $\sigma_0 = 0$ at the crack tips (E and ν - elastic constants). Of course, $r(x, t)$ vanishes along the grain boundary outside the cavities, which are periodically distributed. Elimination of δ from these equations yields the integral representation of the stress distribution. The stress-free boundary condition on the crack surfaces leads to the integral equation for the dislocation density supply rate. The solution for single dislocation on the grain boundary has been obtained and this

solution has been used in this integral representation. The integral equation has been solved numerically for the case of cyclic loading. This solution depends on the dimensionless parameter $\lambda = a[4(1-\nu^2)\omega/ED]^{1/3}$ ($2a$ is crack length, ω is the frequency of the applied load). The parameter λ can be interpreted as the ratio of a crack half-length to a diffusion penetration distance associated with the loading frequency, ω ; however, it is more meaningful to define the diffusion penetration distance, d , to be associated with the loading cycle. Thus, $\lambda = (2\pi)^{1/3} a/d = 1.84 a/d$, and d is a measure of the size of the region extending from the crack tip in which the stress concentration has been relieved by adding material from the crack surfaces during the cycle. In other words, d is the approximate distance between the crack tip and the location of maximum stress acting on the grain boundary. (This interpretation is well supported by computed results.)

In analysis of the stress distribution on grain boundaries for periodically-distributed cracks, it is useful to consider the ratio d/L , where L is half the distance between adjacent crack tips. This ratio represents the relative location of the maximum stress acting on the grain boundary. Thus, for cases with equal values of $\lambda L/a$, the stress fields will look alike.

Important estimations of the stress patterns can be obtained; thus, for values $\lambda L/a > 1.84$, the maximum stress occurs somewhere near the crack tip (at a distance $\frac{d}{L} \approx 1.84 \frac{a}{\lambda L}$). For values $\lambda L/a \leq 1.84$, the maximum stress is at the mid-point and the stress distribution will be parabolic; this is the most relaxed stress field that will occur. The corresponding displacement fields are characterized by the ratio $\frac{\lambda L}{a}$ as well. For values of $\frac{\lambda L}{a} > 2.3$, there is no rigid grain separation and

only the particles in the regions near the crack tips are oscillating; but for smaller values of $\lambda L/a$, rigid separation will begin and all particles on the grain boundary will oscillate. The critical value 2.3 is higher than the value of 1.84 which one would expect, but it is related to the fact that during the part of the period when the remote stresses are decreasing, some time is required before the direction of the matter flux changes. The values of the actual frequencies for various materials at temperature $0.5 T_m$ and for $a = 1\mu m$ are given in Table 4.2 for $\lambda = 5, 20$ and 50 .

Using results for oscillating loads and employing Fourier expansions, the stress and displacement fields have been obtained for step and ramp loadings. For the suddenly-applied loading, results demonstrate that the elastic stress concentrations are effectively relaxed by diffusion after time $t = 0.05\tau$, where $\tau \approx L^3/DE$. By $t = 0.25\tau$ the stress distribution becomes essentially identical to that for rigid grains; i.e., diffusion has become of the dominant process. The values of τ based on the values of crack length $2\mu m$ and crack spacing $20\mu m$ are given in Table 4.2. The typical stress distributions at different instants of time are given in Fig. 4.3. This result can be generalized for any crack spacing to crack length ratio if one considers development of diffusive penetration distance, d/L , in time after step loading has been applied. The approximate expression for this quantity has been obtained.

The analysis of the stress distributions during linear loading demonstrates that for the low loading rate there is no essential elastic stress concentration. On the basis of these results, the practical "safe" load rates can be estimated. Another result which is important for

applications is the displacement response as a function of time. This response for the step and ramp loadings is represented in Fig. 4.4 by the displacement at the middle point between adjacent crack tips on the grain boundary.

(Staff: A. Needleman, J. R. Rice, A. Rubinstein and T. L. Sham)

Table 4.1

γ	E (% error)
1.0	38.4
1.05	34.5
1.10	31.3
1.15	28.0
1.20	24.8
1.25	21.7

$$E \equiv (\dot{V}_{\text{approx}} - \dot{V}_{\text{num}}) / \dot{V}_{\text{approx}} \times 100$$

Accuracy of Eq. (3) as compared to the numerically computed values. The maximum percentage error among all a/L values that are less than 10 is quoted for each γ .

Table 4.2

	$\frac{\omega}{2\pi}$ (cps) for			
Material	$\lambda = 5$ $d = 0.37\mu\text{m}$	$\lambda = 20$ $d = 0.09\mu\text{m}$	$\lambda = 50$ $d = 0.037\mu\text{m}$	τ (H)
FCC				
Nickel	0.4	25.5	400.	2.53
Copper	0.04	2.52	39.4	25.5
Silver	0.09	5.7	90.4	11.1
Aluminum	0.02	1.22	19.2	52.4
Lead	1.4×10^{-4}	9.1×10^{-3}	0.14	7034. (293.1D)
BCC				
Tungsten	5.3×10^{-3}	0.34	5.3	190.0
Chromium	2.9×10^{-3}	0.19	2.9	344.0
Molybdenum	0.02	1.42	22.2	45.3
Alpha Iron	0.1	6.62	103.5	9.73
HCP				
Zinc	0.016	1.01	15.9	63.4
Magnesium	0.17	11.0	173.	5.82

Data for $T = 0.5T_m$ and $a = 1\mu\text{m}$

$$\omega(T) = \omega(0.5T_m) \cdot \frac{0.5T_m}{T} e^{Q_b [2 - T_m/T]/RT_m}$$

$$d = \frac{1.84}{\lambda} \mu\text{m}$$

J_b - atom flux rate on grain boundary

Ω - atomic volume

$$b/a = 10$$

$$h/a = 10$$

$$\psi = 70^\circ$$

Figure 4.1

Figure 4.2

Figure 4.3

Figure 4.4

B. REPORTS, PUBLICATIONS, ORAL PRESENTATIONS, THESES AND DEGREES AWARDED

1. Technical Reports

COO-3084-79 Progress Report (June 1980)

COO-3084-80 L. Majno and R. Asaro, Grain Refining and High Temperature Austenitization of 4340 Steel and Their Effect on Microstructure and Mechanical Properties (February 1981)

COO-3084-81 S. Kubo, Effects of Creep Recovery and Hardening on the Stress and Strain-Rate Fields Near a Crack Tip in Creeping Materials (December 1980)

COO-3084-82 H. Cialone and R. Asaro, Hydrogen Effects in the Cracking of High Strength 4140 Steel (March 1981)

COO-3084-83 J. Gurland, Load Transfer in a Dual-Phase Steel (June 1981)

2. Publications

H. Cialone and R. J. Asaro, "Hydrogen Assisted Fracture of Spheroidized Plain Carbon Steels", Metallurgical Transactions, in press.

*H. Cialone and R. J. Asaro, "Hydrogen Assisted Fracture of Spheroidized Plain Carbon Steels", Proceedings of the Third International Conference on the Effect of Hydrogen on Material Behavior, AIME pub., ed. A. W. Thompson and I. M. Bernstein.

*J. R. Fisher and J. Gurland, "The Effect of Alloy Deformation on the Average Spacing Parameters of Non-Deforming Particles", Metallurgical Trans. A, (1981) 12A, 167-171.

J. R. Fisher and J. Gurland, "Void Nucleation in Spheroidized Carbon Steels, Part I: Experimental Study" Metal Science (in press)

J. R. Fisher and J. Gurland, "Void Nucleation in Spheroidized Carbon Steels, Part II: A Comprehensive Model" Metal Science (in press)

*A. Needleman and J. R. Rice, "Plastic Creep Flow Effects in the Diffusive Cavitation of Grain Boundaries", Acta Metallurgica, 28, 1981, pp. 1315-1332 (Overview No. 9).

J. R. Rice and Tze-jeer Chuang, "Energy Variations in Diffusive Cavity Growth", Journal of the American Ceramic Society, 64, 1981, pp. 46-53.

J. R. Rice, "Elastic-Plastic Crack Growth", in Mechanics of Solids: The Rodney-Hill 60th Anniversary Volume, ed. H. G. Hopkins and M. J. Sewell, Pergamon (in press).

* Previously listed as "in press" or "submitted"

3. Oral Presentations and Seminars

J. Gurland

Fall Meeting of AIME, Pittsburgh, PA, October 1980, presented papers on (1) The Effect of Alloy Deformation on Average Spacing Parameters of Non-Deforming Particles and (2) Void Nucleation at Hard Particles.

Reed Tool Co., Houston, Texas, March 1981, research seminar on fracture of steels and cemented carbides.

R. J. Asaro

Third International Conference on the Effect of Hydrogen on Behavior of Materials, Jackson Lake, Wyoming, August 1981, "Hydrogen Assisted Fracture in Plain Carbon Steels"

H. Cialone

"Hydrogen Assisted Fracture of Spheroidized Plain Carbon Steels", General Electric Research, Schenectady, NY, October 1980.

"Hydrogen Assisted Fracture of Spheroidized Plain Carbon Steels", Carrier Corp. Research Laboratories, Syracuse, NY, September 1980.

"Hydrogen Effects in the Fracture of Steels", Systems Research Laboratories, Dayton, Ohio, September 1980.

"Effects of Hydrogen on the Fracture of Steels", Brown University, January 1981.

Walter Drugan gave two seminars on

Asymptotic analysis of growing cracks in elastic-ideally plastic solids - Part I : General Formulation (November 1980)
Part II: Specific Solutions for Plane Strain Growth (December 1980)
at Brown University, Providence, Rhode Island.

Asher Rubinstein gave seminars on

"Diffusive Relaxation of the Stress Concentrations on Grain Boundaries"
at Brown University, Providence, R. I. (September 1980)
Drexel University, Philadelphia, Pa. (March 1981)
Northeastern University, Boston, Ma. (March 1981)
Gulf Research Center, Pittsburgh, Pa. (March 1981)
Rockwell International Research Center, Thousand Oaks, California (March 1981)
State University of New York at Stony Brook, N. Y. (April 1981)
M.I.T., Cambridge, Ma. (April 1981)
Boston University, Boston, Ma. (April 1981)

J. R. Rice gave the "Concluding Technical Discussion" at the 5th International Congress on Fracture, Cannes, France (April 1981), gave a lecture on "Creep Cavitation of Grain Interfaces" at the

UTAM Symposium on 3-D Constitutive Relations and Ductile Fracture, Dourdan, France (June 1980), and gave the "Summary Discussion" at the Conference on Shear Localization, Newport, R. I. (August 1980). He also gave a seminar at Brown University on "Elastic-Plastic Crack Growth" during fall 1980.

4. Theses and Degrees Awarded

Theses

H. Cialone, Ph.D. - "Hydrogen Effects in the Fracture of Spheroidized Plain Carbon Steels and a High Strength 4140 Steel", January 1981.

L. Majno, Sc.M. - "Grain Refining and High Temperature Austenitization of 4340 Steel and Their Effect on Microstructure and Mechanical Properties", February 1981.

Degrees Awarded

H. Cialone, Ph.D. - June 1981

L. Majno, Sc.M. - June 1981

C. PERSONNEL

1. Professional Staff: R. J. Asaro, J. Gurland, A. Needleman and J. R. Rice.
2. Research Engineer: L. Hermann.
3. Technical Assistants: W. Rebello and H. Stanton.
4. Research Assistants (Graduate Students): H. Cialone*, W. J. Drugan, L. Majno*, A. Rubinstein, A. Szewczyk and T. L. Sham.
5. Visiting Research Associate: Dr. S. Kubo**
6. Senior Undergraduate Research Assistant: Merrilca Mayo.
7. Employment of Recent Graduates:
Dr. H. Cialone - Battelle Memorial Laboratories,
Columbus, Ohio.
Dr. J. R. Fisher - Western Electric Laboratories,
Princeton, New Jersey.
Mr. L. Majno - Instron Corporation
Canton, Massachusetts.

* Supported for portion only of contract period.

** Not supported by contract.